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SOFTWARE USER'S MANUAL FOR THE RAILCAR4.1 TOXIC INDUSTRIAL CHEMICAL SOURCE CHARACTERIZATION PROGRAM

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ASYMMETRIC SYSTEMS DEPARTMENT

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This document discusses the use of the RAILCAR4.1 Toxic Industrial Chemical Source Characterization Program to analyze a scenario in which there is a release of a toxic industrial chemical from a transport or storage tank, such as chlorine released from a rupture in a 90-ton railcar. The RAILCAR4.1 program addresses a knowledge gap associated with releases of pressurized liquid by providing an accurate characterization of the vapor source resulting from the liquid jet. The mist pool theory underlying the RAILCAR4.1 pressurized liquid source characterization was validated by the Jack Rabbit pilot tests and field trials, and the program was calibrated to match measured data. RAILCAR4.1 also predicts source terms for other chemicals that result in plumes or boiling or evaporating liquid pools. RAILCAR4.1 expands upon RAILCAR4 by adding a graphical user interface and providing output that can be entered into hazard assessment models used by emergency responders to better protect the public and warfighters from these types of incidents.

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FOREWORD

This document discusses the use of the RAILCAR4.1 Toxic Industrial Chemical Source Characterization Program to analyze a scenario in which there is a release of a toxic industrial chemical from a transport tank, such as chlorine released from a rupture in a 90-ton railcar. The RAILCAR4.1 program addresses a knowledge gap associated with releases of pressurized liquid by providing an accurate characterization of the vapor source resulting from the liquid jet. The mist pool theory underlying the RAILCAR4.1 pressurized liquid source characterization was validated by the Jack Rabbit pilot tests and field trials, and the program was calibrated to match measured data. RAILCAR4.1 also predicts source terms for other chemicals that result in plumes or boiling or evaporating liquid pools. RAILCAR4.1 expands upon RAILCAR4 by adding a graphical user interface and providing output that can be entered into hazard assessment models used by emergency responders to better protect the public and warfighters from these types of incidents.

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GLOSSARY

AEGL	Acute Exposure Guideline Level
ATD	Atmospheric Transport and Dispersion
ATM	Atmosphere
CSAC	Chemical Security Analysis Center
CSG	Challenge Sub-Group
DHS	Department of Homeland Security
DoD	Department of Defense
DOT	Department of Transportation
DPG	Dugway Proving Ground
FFI	Norwegian Defense Research Establishment
GUI	Graphical User Interface
JECP	Joint Expeditionary Collective Protection
LNG	Liquefied Natural Gas
LPG	Liquefied Propane Gas
MDA	Modelers' Data Archive
NATO	North Atlantic Treaty Organization
NSWCDD	Naval Surface Warfare Center Dahlgren Division
OHA	Operational Hazard Analysis
SME	Subject Matter Expert
S&T	Science and Technology
TIC	Toxic Industrial Chemical
TIM	Toxic Industrial Material
TSA	Transportation Security Administration
U.S.	United States
VLSTRACK	(Chemical and Biological Agent) Vapor, Liquid, and Solid Tracking

1   INTRODUCTION

On 6 January 2005, a train wreck in Graniteville, South Carolina, led to the rupture of a 90-ton chlorine railcar resulting in the release of 54 tons of chlorine.[1] Over 5,000 people in the lightly populated area were evacuated; over 500 people sought medical treatment; nine (9) people died. This accident led to concern among city planners, emergency responders, the transportation industry, the chemical industry, the Department of Homeland Security (DHS), and the Department of Defense (DoD) about potential attacks on chemical railcars and tanker trucks transiting an urban area, or chemical storage tanks near an urban area. A comparison of modern hazard assessment model predictions at the time consistently suggested that lethal concentrations from large releases of chlorine would persist within the plume of toxic vapor beyond six miles downwind.[2] Modeling results indicated that hundreds of thousands of persons would need to be evacuated as the plume spread rapidly through the urban area.

Such a large evacuation effort would be impractical for emergency responders in terms of both resources and time. Further, records of toxic effects from accidents like that in Graniteville suggest the downwind hazard area is much shorter than the hazard assessment models predict. The nine deaths in Graniteville all occurred within half a mile of the accident. The World War I Battle of Ypres, France, on 22 April 1915 involved release of chlorine from several thousand cylinders along a four-mile-long trench, but deaths were limited to within less than one half mile of the release trench.[3] Even the over 2,000 deaths in Bhopal, India, which resulted from the 3 December 1984 release of 40 tons of methyl isocyanate, occurred within less than two miles; the large number of deaths were associated with the high population density rather than the downwind distance of that highly toxic chemical.[4]

To address the large discrepancy between recorded toxic effects and model predictions, the Transportation Security Administration (TSA) assembled a group of subject matter experts (SMEs) from the chemical industry, transportation industry, national labs, academia, emergency response organizations, DHS, DoD, and the intelligence community. A meeting was held on 8-9 November 2006 in McLean, Virginia, and was co-chaired by this document's author from the Naval Surface Warfare Center, Dahlgren Division (NSWCDD).[5] Discussions focused on the release of chlorine from a 90-ton railcar and the identification of knowledge gaps associated with such a release. The most important knowledge gaps fell into three (3) categories: 1) characterization of the vapor source resulting from the liquid jet, 2) human toxic effects, and 3) reaction of the chlorine vapor with and removal by surfaces and air as it travels downwind. Each is discussed below.

1.1   Vapor Source Characterization

Survivors of the Graniteville accident reported that chlorine vapor remained in the release area for at least two (2) hours. The chlorine vapor plume also followed the path of the valley within which Graniteville is located, which was somewhat different from the wind direction at the time of the accident. The chlorine was thus heavily influenced by the terrain features, along with the buildings and vegetation in the release area. Conversely, hazard prediction models all assumed that the liquid jet would mix with passing air and be carried downwind as a long vapor plume. These modeling approaches agreed with data from field trials involving large releases of Toxic Industrial Chemicals (TICs), such as ammonia; but those releases occurred over flat desert terrain under a fairly high wind speed. Field trials were limited by available test sites and the requirement that the wind direction remain steady and predictable for safety reasons.[6]

One theory addressing these additional features, developed by the author in 2008, was that large TIC masses of vapor and aerosol released over a short time period would pool into a large cloud at the release site and give off vapor into the passing air over an extended time period.[7] This pooling was likely enhanced by the presence of buildings, vegetation, and terrain depressions in the release area. The significance of having a long-duration source of vapor instead of a short-duration plume was that the concentration of the chemical downwind of the release site was lower and less toxic, especially when coupled with the human toxic effects described in the next section. TIC vapor plume formation versus pooling at the release site is shown in Figure 1.
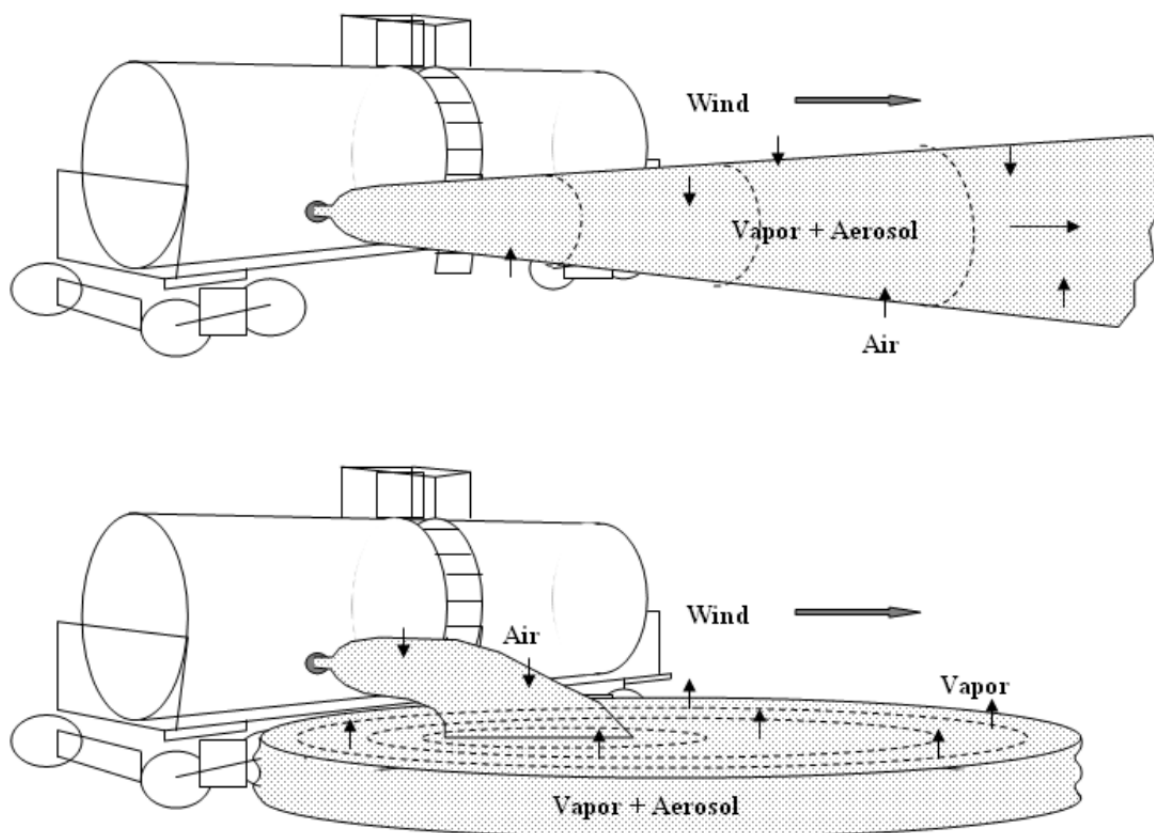
Figure 1. TIC Vapor Plume Formation Versus Pooling at the Release Site

1.2 Human Toxic Effects

The model predictions used to estimate the downwind hazard areas were based on chemical concentrations called Acute Exposure Guideline Levels (AEGLs) developed for the Environmental Protection Agency.[8] For a given chemical, there are AEGLs for life-threatening, serious, and irritating effects. Human toxic responses are a function of exposure (which combines concentration and duration), rather than just concentration, so there are AEGLs for a range of exposure durations ranging from 10 minutes to eight (8) hours. The problem with the AEGLs identified by the SMEs was that they were set for the most sensitive subpopulation rather than the average person. Thus, the AEGLs cannot be used to estimate expected casualties from a TIC incident.

An important aspect of human toxic responses is that, for one-time acute exposures, the human body can slowly expel or otherwise counter a toxic chemical. A high concentration received over a short duration, therefore, is more toxic than an equivalent exposure involving a low concentration over a longer time period. This "toxic load" approach reveals why lowering the vapor concentration at the release location, as discussed above, can dramatically reduce the size and length of the downwind hazard area. Even if the TIC does travel downwind as a high concentration plume, use of higher toxicity values appropriate for the average person and

the toxic load approach with existing hazard prediction models will greatly improve model output.

The importance of proper source characterization and toxicity estimation can be demonstrated using a hypothetical scenario involving release of a TIC. Figure 2 shows the number of persons requiring medical attention (i.e., casualties) using three (3) common hazard area representations: circle, fan, and contour. The population density is assumed uniform, so casualties reflect relative areas within each representation. The radius of the circle and fan and the length of the contour are the same and represent the current AEGL approach. Casualties ranged from 1,288 within the model contour to 22,182 if a simple circle is drawn. If the toxic load approach is then used with the same model output but using toxicity values for the total population distribution (as opposed to the most sensitive subpopulation), the length of the contour decreases considerably, and the number of casualties drops to 32, as shown in Figure 3.

1.3   Reaction and Removal Mechanisms

Reaction of the TIC vapor with surface materials such as concrete and metal, reaction with water vapor and air pollutants, and absorption into the surface materials at the release location all act to decrease the TIC mass traveling downwind, resulting in lower concentrations and reduced downwind toxic effects. The chlorine vapor at Graniteville penetrated the ground at the release site and had to be neutralized with large amounts of lime. As the chlorine vapor traveled downwind, it corroded exposed metal surfaces such as doorknobs and electrical transformers. The vapor reaction with surface materials formed a different compound, pulling mass out of the vapor plume and lowering its concentration. Chlorine vapor was also absorbed into porous materials such as building insulation. One issue with absorption is that, once the plume has moved on, the TIC may then desorb from within the surface. This process would result in a low concentration over an extended time period and reduced toxic effects, but not a lower total vapor mass. Although some TIC reaction data exists, the data were generated for pollution monitoring purposes using very low TIC concentrations rather than the high concentrations relevant to incidents. Data are still needed on how fast and how far the relevant reactions will occur to estimate the mass removed from the plume as it travels downwind.
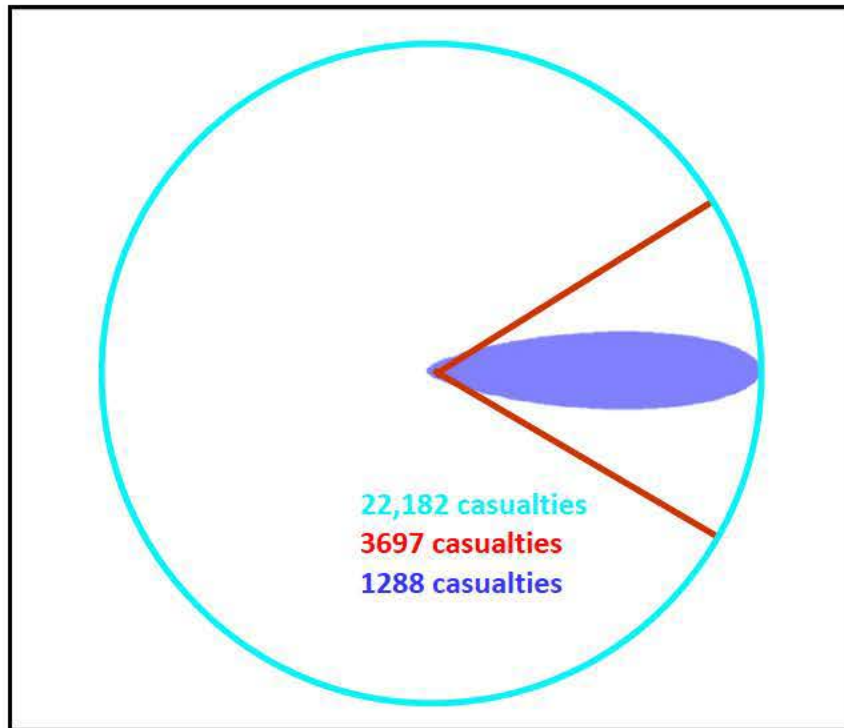
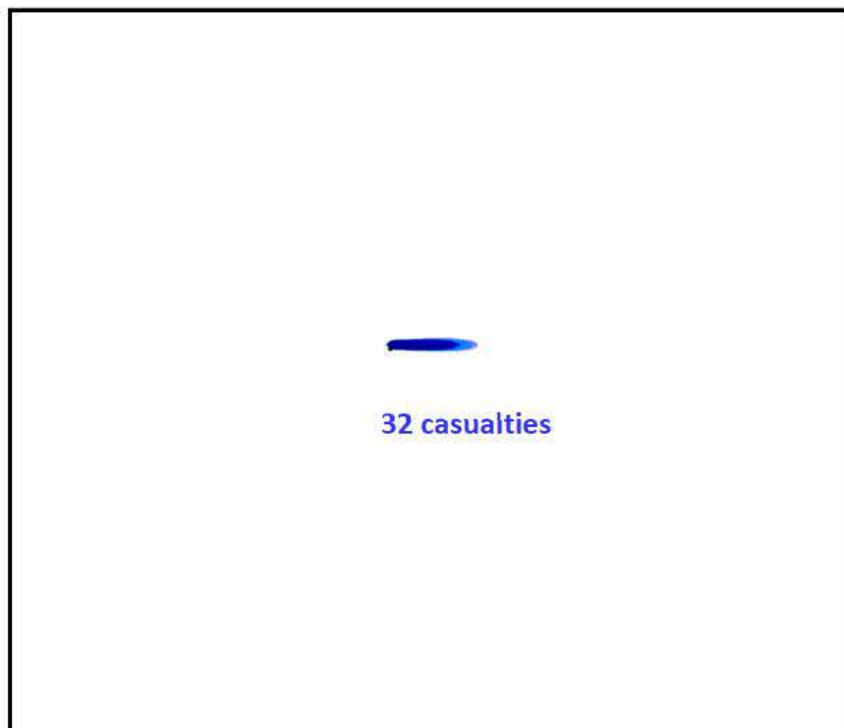**Figure 2. Hypothetical TIC Incident Common Casualty Estimation Approaches**

Figure 3. Hypothetical TIC Incident Toxic Load Casualty Estimation Approach

2   RAILCAR PROGRAM DEVELOPMENT

The mist pool theory published by Bauer and Fox[7] through the DHS Chemical Security Analysis Center (CSAC) is:

> Under low to moderate wind speeds, if the mass flow of a pressurized liquid jet exceeds the capacity of the passing air to entrain it, the vapor and aerosol will form a stationary cloud or "mist pool" at the release location and result in an area source vapor flux; mist pool behavior is enhanced by the presence of buildings, vegetation, and terrain depressions.

The significance of having a mist pool form in place of a plume from the two-phase jet is that the lower vapor concentrations, when combined with toxic load values, lead to greatly reduced downwind hazard distances that are consistent with incident observations.

Bauer and Fox[7] define a single criterion to determine if a mist pool will form:

$$Q_v/Q_j = 2.87\ B\ C\ u_*\ \pi\ D_c^2/(8\ Q_j\ Ri_*\ ) < 1 \qquad [1]$$

$$D_c = [4\ Q_j\ (1 + E\ \rho_{air}/\ \rho_J)/\pi\ \rho_c\ H_c]^{0.5}\ t^{0.5} \qquad [2]$$

$$Ri_* = g\ (\rho_c - \rho_{air})\ H_c/\ \rho_{air}\ u_*^{\ 2} \qquad [3]$$

Where Q_v is the vapor mass entrainment rate, Q_j is the jet mass flow rate, C is the mist pool concentration, u_* is the friction velocity for the ambient wind conditions, π is the constant pi, D_c is the mist pool diameter, Ri_* is the friction-velocity-based Richardson number, E is the volumetric air entrainment ratio equal to the volume of air mixed into the jet over the volume of the jet, ρ_{air} is the ambient air density, ρ_J is the jet density, ρ_c is the mist pool density after air entrainment, H_c is the mist pool height or thickness, t is the tank empty time, and g is the gravitational acceleration constant (9.81 m/s^2). B is an entrainment factor set to five (5) if entrainment is enhanced by the jet aiming upwards or with the wind or the terrain is flat and smooth, as was typical for the desert field trials mentioned above. B is set to 0.2 if entrainment is inhibited by the presence of buildings, vegetation, and/or terrain undulations at the release location that shelter the jet from the ambient wind. B is set to one (1) if entrainment is neither enhanced nor sheltered.

In order to estimate the vapor mass entrainment rate, a mist pool must be assumed to form using the TIC mass released in the jet. Jet mass flow rate and tank empty time are computed

from the size of the hole in the tank and calculations of the thermodynamic behavior of the TIC vapor and liquid inside the tank as it empties. Mist pool concentration and density are computed from the TIC and air component properties. Friction velocity is estimated using empirical relations involving the surface air velocity, the amount of turbulence in the surface layer, and a characterization of the roughness of the surface. The mist pool height is assumed to be one (1) to two (2) m, based on field trial and accident observations of the thickness of dense gas clouds after they have stabilized. The volumetric air entrainment ratio is also an assumed value, thought to range between five (5) and 20 for typical two-phase jets. Jet density is determined from an adiabatic expansion energy balance where the jet cools to the TIC boiling temperature by vaporizing liquid. These properties then allow the mist pool diameter and Richardson number to be computed. The factor of eight (8) in Equation (1) comes from estimating the average cloud area during formation as half of the final cloud area of $\pi D_c^2/4$.

Since the equations for these parameters can be quite complex, the RAILCAR program was written to compute all values needed for the mist pool formation criterion, as well as the subsequent mist pool behavior. Bauer and Fox[7] provide methodology for the following processes:

- Tank thermodynamics during emptying
- Jet velocity and flow rate
- Jet expansion to ambient pressure
- Plume equilibrium following air entrainment
- Mist pool formation criterion

If the mist pool criterion is not met (i.e., the vapor entrainment to jet ratio is greater than or equal to one (1)), the source becomes a plume with the temperature, density, concentration, and duration computed using this methodology. The plume characteristics can be entered into a transport and diffusion model as a stationary vapor or two-phase point source. There are proprietary codes that contain sophisticated algorithms for the first four (4) of these processes and the subsequent plume transport and diffusion, but those models do not consider the different source characteristics resulting if a mist pool forms.[9,10]

If the mist pool criterion is met, Bauer and Fox[7] provide vapor flux methodology for the transition points of a mist pool:

- At the tank empty time
- When all liquid aerosol has evaporated
- When the Richardson number drops to 12
- When the Richardson number equals zero (0)

The change in mass and average vapor flux between each of these transition points can be used to determine the duration of each mist pool stage, with the total mist pool duration being the

sum of the times. The mist pool characteristics must then be entered into a transport and diffusion model as an area vapor source.

The above methodology was converted into computer algorithms as the RAILCAR program. The program name was assigned based on the original goal of the TSA-initiated effort to estimate the source conditions and subsequent transport and diffusion of chlorine released from a 90-ton railcar. RAILCAR originally only contained thermodynamic properties for chlorine and was limited to chlorine railcar, transport truck, and one-ton shipping tanks. The thermodynamic properties of anhydrous ammonia were then added to allow for comparison of these two (2) most commonly shipped TICs. RAILCAR does not compute TIC transport and diffusion.

2.1   RAILCAR Studies and Analyses

Multiple DoD, DHS, and international organizations are interested in estimating the toxic hazard areas resulting from TIC incidents. The Toxic Industrial Chemical/Toxic Industrial Material (TIC/TIM) Task Force was established by the Joint Program Executive Office for Chemical and Biological Defense in 2007 to develop a prioritized list of TICs. The Task Force determined the relative ranking of over 400 TICs and arrived at a list containing the highest ranked chemicals, which was further reduced to 16 priority TICs.[11] The toxicity, volatility, and shipping quantities of these TICs led to their rankings, but it was still to be determined if they could be released in a manner leading to a large downwind inhalation/ocular hazard area.

DHS CSAC developed a similar list of TICs of concern for homeland security. The ones relevant to inhalation toxicity overlapped considerably with the DoD list. DHS Science and Technology (S&T) directorate funding allowed the thermodynamic properties of 42 chemicals to be added to chlorine and ammonia in RAILCAR.[12] Thirty-nine (39) of the 49 total chemicals are the highest ranking ones from the TIC/TIM Task Force and include chlorine and anhydrous ammonia. The remaining chemicals are:

- Acrolein — considered a priority TIC by the North Atlantic Treaty Organization (NATO) Challenge Sub-Group (CSG)
- Ethylene Oxide — of TSA and industry concern as both a toxic and explosive downwind hazard
- 1,1,1,2-tetrafluoroethane (R134) — a refrigerant having potential as a chlorine and ammonia simulant
- Dichloromethane — an organic solvent for pesticide dispersal
- Water — a solvent for TICs in aqueous solution (e.g., ammonium hydroxide, hydrofluoric acid)
- Dinitrogen tetroxide — the dimer of nitrogen dioxide that is a TSA high transport volume chemical of concern
- Acrylonitrile — a TSA high transport volume chemical of concern

- Freon-12 (dichlorodifluoromethane) — a refrigerant used in the Thorney Island dense gas field trials, as summarized in the Modelers' Data Archive (MDA)[13]
- Methane (liquefied natural gas (LNG)) — a flammable chemical used in the Burro, Coyote, and Maplin Sands dense gas field trials, as summarized in the MDA
- Propane (liquefied propane gas (LPG)) — a flammable chemical used in the Maplin Sands dense gas field trials, as summarized in the MDA

The last three (3) chemicals have been added to validate coupled RAILCAR-atmospheric transport and dispersion (ATD) models against the dense gas field trials included in the MDA, which was created for dense gas ATD model validation. The list of TICs for which thermodynamic properties are available for RAILCAR is included in Table 1.

Table 1. TICs Available for RAILCAR Simulations

acetylene tetrabromide	formaldehyde	o-anisidine
acrolein	Formalin (37%)	OMPA
acrylonitrile	Freon-12	parathion
ammonia	hydrobromic acid (48%)	phosgene
ammonium hydroxide (29%)	hydrochloric acid (39%)	phosphine
arsine	hydrofluoric acid (38%)	phosphorus trichloride
boron trifluoride	hydrogen bromide	phosphoryl trichloride
bromine	hydrogen chloride	propane (LPG)
chlorine	hydrogen cyanide	sulfur dioxide
chlorine dioxide	hydrogen fluoride	sulfuric acid
cyanogen chloride	hydrogen sulfide	sulfur trioxide
dichloromethane	malathion	1,1,2,2-tetrachloroethane
dinitrogen tetroxide	mercury	1,1,1,2-tetrafluoroethane
ethylene dibromide	methane (LNG)	toluene-2,4-diisocyanate
ethylene oxide	methyl bromide	water
fluorine	nitric acid	
fluorotrichloromethane	nitrogen dioxide	

The DHS S&T task also allowed for additional RAILCAR algorithm development to address processes associated with TICs having lower volatility, such as liquid pool evaporation. Again, other models contain similar algorithms, but RAILCAR is the only program that combines these source characterizations in a single model.

RAILCAR was used as part of a TIC/TIM Task Force operational hazard analysis (OHA) to provide source characterization for vignettes to determine the potential hazard of these TICs if released in an attack against forward deployed troops.[14] RAILCAR has also been used for a second OHA that addresses limitations identified with the first OHA and includes vignettes for additional priority TICs. RAILCAR was used to estimate the source characteristics for six (6) chlorine

vignettes and one (1) acrolein vignette for a NATO CSG study that provides concentration challenge levels to NATO protective equipment.[15] The program was used in a study for the Joint Expeditionary Collective Protection (JECP) acquisition program to characterize the sources for chlorine and sulfur dioxide vignettes for evaluating JECP shelter performance for proposed designs.[16] RAILCAR was also used to characterize the source for the TSA for potential chlorine and ethylene oxide railcar attacks in urban areas and as part of a Navy shipboard threat study involving attacks on Navy ships in port using six (6) different TICs.

2.2   The RAILCAR Validation Issue

The mist pool theory, as defined in the Bauer and Fox[7] report, was reviewed by members of the TSA group of SMEs prior to publishing. CSAC also funded external reviews. The theory was found credible; however, at the time there were no data involving formation of a mist pool from release of a pressurized liquid. What did exist were observations from accidents and attacks. Observers of the Graniteville accident reported patches of chlorine hanging around the release location for at least two (2) hours.[1] Some of the chlorine from the Ypres cylinders settled into the downwind trenches where it remained well beyond when the bulk of the plumes had dissipated.[3] The chlorine transfer line rupture in Festus, Missouri, was near a row of trees that effectively prevented chlorine from passing to the other side.[17] In addition, field trials, wind tunnel, and water chamber tests involving releases of denser-than-air (or denser-than-water) materials under very low flow conditions were identified by the TSA SMEs, which showed stationary cloud formation and/or detrainment of mass into the air/water flow above. The vapor mass entrainment rate equations, in Section 2 above, were selected from three (3) sources that had already proposed algorithms dealing with creation of a stationary vapor cloud above a boiling liquid pool.[18-21]

Since none of the trials involved formation of a mist pool under more moderate wind speeds from release of a pressurized liquid, comparison of the RAILCAR mist pool methodology to data could only involve showing that the test conditions did not meet the mist pool formation criterion. The ammonia releases of the Desert Tortoise field trials do not meet the criterion.[22] The United States (U.S.) Army conducted the Wild Stallion field trials at Dugway Proving Ground (DPG) releasing chlorine from one (1)-ton tanks in October 2007.[23] These tests were conducted in response to the attacks in Iraq employing similar one (1)-ton chlorine tanks.[24] Although parts of the resulting chlorine clouds and plumes did remain at the release location for up to 30 seconds, RAILCAR predicts a much longer mist pool duration. In order to validate both the mist pool theory and the RAILCAR program, new data are needed.

2.3   Jack Rabbit Test Program

The most significant effort to date to generate data necessary to improve downwind hazard area estimation was the set of field trials conducted at DPG during the period 27 April through 21 May 2010. Pilot tests of ammonia and chlorine releases were conducted on 7 and 8 April,

respectively. Funding was provided by TSA and managed by the Edgewood Chemical Biological Center. The project was operated by CSAC, and the trials were conducted by DPG.[25] The test design (Figure 4) was created by NSWCDD and the Norwegian Defense Research Establishment (FFI).
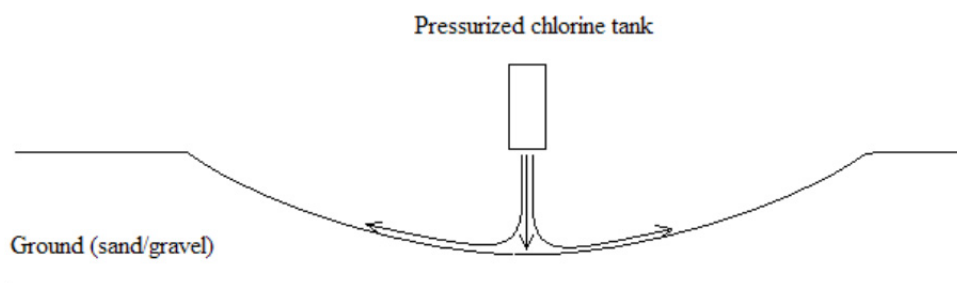

Figure 4. Jack Rabbit Test Design

NSWCDD and FFI took advantage of an existing collaborative effort to work on the Jack Rabbit Test Program. The field trials were intended to prove or disprove the NSWCDD theory regarding the pooling of chlorine (or other TICs transported as pressurized liquids) vapor and aerosol at the release location, so the design included a circular pit designed to shelter chlorine and ammonia against the wind flowing over it. The goal was to have a tank empty time of 30 seconds and mist pool duration of five (5) minutes. RAILCAR and other jet models were used to determine the hole, pipe, and valve sizes. RAILCAR projected that a wind speed of two (2) to three (3) m/s under stable conditions or one (1) to two (2) m/s under neutral conditions would result in the five (5)-minute mist pool duration. The test geometry was refined by FFI using computational fluid dynamics modeling.[26] Instrumentation was specified and positioned by the TSA group of SMEs. Four (4) trials each were conducted with chlorine and ammonia involving the rapid release of two (2) tons of liquid directed downward into the pit. The same tanks were used for the two (2) pilot tests, but the tanks were only filled with one (1) ton of each TIC. NSWCDD and FFI provided on-site modeling and analysis support during the trials. The trials did result in chlorine and ammonia pooling in the pit and releasing vapor into the passing air, validating the mist pool theory (see Figure 5). As described below, however, additional algorithms had to be developed and added to RAILCAR to be able to simulate the ammonia and chlorine behavior. By adjusting several input parameters, good agreement with data was obtained. However, as the Jack Rabbit field trial data were used to adjust the model, additional field trials are now needed to validate the program.

Ammonia Pilot Test at <10 sec

Chlorine Pilot Test at <10 sec

Ammonia Pilot Test at 3 min

Chlorine Pilot Test at 3 min

Figure 5. Jack Rabbit Ammonia and Chlorine Video Images (extracted from DPG videos)

2.4   New Algorithm Development and Adjustment

The methodology defined by Bauer and Fox[7] and coded as the original RAILCAR program was insufficient to simulate the ammonia and chlorine Jack Rabbit field trials. New algorithms were developed and existing ones adjusted during the trial period. The resulting RAILCAR2 program was able to match key parameters measured during the field trials. The rapid code changes made the source code quite unstructured, so the source code was rewritten in a modular fashion after completion of the test program. The algorithms and their operation were verified by the author. The result was the RAILCAR3 program.

The tanks had three (3) characteristics not addressed by the mist pool theory methodology. First, the mist pool theory assumed the tank to be completely full of liquid. Real transport and storage tanks, and the Jack Rabbit tanks after filling, have a vapor space above the liquid called ullage. The initial tank conditions, therefore, have both liquid and vapor present. Second, the air in the empty tanks is displaced to some extent during the filling process, but much of the air is trapped and compressed into the ullage volume. Industry will also add nitrogen to pressure

tanks to make sure that rupture disks and relief valves are within their proper pressure range. Third, SME concerns over vaporization within the pipes and values attached to the tank bottom led to restrictor orifices being constructed. A vapor phase was added to the algorithms for initial tank conditions, which had to be carried through the tank-emptying algorithms. An inert vapor phase was likewise added to the same set of algorithms. The jet mass flow algorithms were modified by adding the area ratio of the orifice to the inner pipe/valve and assuming no additional frictional losses. The RAILCAR program also had a lower limit of 0 °C for the tank and air temperatures, and had to be lowered for the test conditions.

Once the pilot tests and field trials began, a series of "significant observations" required additional RAILCAR algorithm development and modifications. The most significant of these observations was that the volumetric air entrainment ratio was much higher than the assumed range of five (5) to 20. Based on the final cloud diameter and thickness and the measured cloud temperature, the volumetric air entrainment ratio ranged from 100 to 290. The much higher volume of air entrained into the jet was not only sufficient to evaporate all aerosol, but it then raised the cloud temperature above the ammonia and chlorine boiling temperature characteristic of the jet after adiabatic expansion but prior to air entrainment. The disappearance of the aerosol was evident in the chlorine videos, where the white aerosol disappeared beyond about 10 m from the tank. The mist pool theory was affected by this observation in that the two (2)-phase mist pool was replaced by a vapor phase stationary cloud. The mist pool methodology assumed that aerosol was present, so new RAILCAR algorithms had to be developed to address the energies of aerosol evaporation and cloud warming. In a real-world incident involving a large tank of pressurized liquid, it is likely that the volumetric air entrainment ratio will be in the range of the Jack Rabbit field trial observations rather than the original values derived from small-scale tests. As the Jack Rabbit field trials show, stationary clouds will still form under suitable release and environmental conditions, but the much lower cloud density will result in cloud durations shorter than those from a low entrainment ratio. Note that RAILCAR3 will still predict the formation and behavior of a two (2)-phase mist pool if the volumetric air entrainment ratio is low enough.

The next significant observations affected the jet and tank empty times. The mist pool methodology assumes that there will be a transition between an all-liquid jet and an all-vapor jet when the vapor-liquid interface within the tank reaches the hole. The depressurization of the tank occurs in a much shorter time period than the liquid empty time. The methodology only allows vaporization within a pipe attached to the tank if the frictional pressure loss in the pipe exceeds the liquid head pressure within the tank. The Jack Rabbit field trial data and videos had slower liquid mass flow rates than predicted and similar liquid empty and depressurization times. The slower liquid mass flow rate was evidence that the liquid in the pipe was vaporizing before the orifice, and the extended depressurization time suggested that the liquid in the tank foamed in the vapor space. The RAILCAR jet algorithms were modified to allow vaporization within the pipe even if the frictional losses do not exceed the liquid head pressure and to use a two (2)-phase density for the depressurization phase. In a real-world incident, foaming is likely to occur if the hole is large (e.g., at least two (2) inches in diameter). Vaporization is only relevant if the incident involves a break in a pipe attached to the tank.

Another significant observation was that there was much "rainout" of the aerosol in the jet due to impaction with the steel plate two (2) m below. The INERIS test program included tests of ammonia jets impacting horizontal barriers three (3) m or less from the nozzle. In some cases, more than 50 percent (%) of the ammonia "rained out" onto the ground surface below the barrier.[27] The pool diameter observed in the videos and from the subsequent appearance of the soil in the pit suggested that six (6) to 60% of the ammonia and chlorine rained out to form a boiling liquid pool. The liquid pool evaporation algorithms in RAILCAR were only used for TICs with boiling temperatures less than 20 °C below the temperature (e.g., the superheat temperature) where large droplets are formed and fall out of the jet. The RAILCAR pool evaporation algorithms were modified to allow pool formation for TICs with higher superheat temperatures. In a real-world incident, rainout of pressurized liquids will occur if the jet impacts the ground, which is likely in an attack aimed at the lower half of the tank. During the pilot tests, the liquid pool disappeared within 10 minutes or less, with no visible off-gassing from the soil. Ice from water vapor did form on the steel plate and surrounding soil, which then melted and disappeared. The pool and ice formation, melting, and evaporation chewed up the soil around the steel plate. Liquid absorbed into the rough and porous soil during all the field trials. Visible off-gassing lasting for up to one (1) hour was observed during the later trials. The RAILCAR algorithms allowed for pool evaporation, but not subsequent off-gassing. The algorithms were modified to allow a fraction of the liquid in the pool to evaporate at a much slower rate following normal evaporation of the rest of the pool. In a real-world incident, absorption into porous materials like soil and concrete is likely. The slower off-gassing can affect emergency responders by requiring them to wear protective gear for extended periods of time in the release area or even conduct extensive decontamination operations. Liquid pools forming on nonporous surfaces like asphalt or even ballast stone will evaporate before the responders are likely to arrive and don protective gear.

The final significant observation was that the temperature in the tank remained almost constant while liquid was present, as predicted by the mist pool theory and other models, but the pressure in the tank dropped considerably lower than predicted. The author proposes that the pressure drop is due to adiabatic expansion of the inert vapor trapped in the ullage space as the vapor space increases over the liquid empty time. The adiabatic expansion leads to a lower temperature in the vapor space than that of the liquid below. Unfortunately, there was only a single thermocouple in the liquid space of the tank; a thermocouple in the vapor space is needed to confirm that temperature is no longer in equilibrium. Adiabatic expansion has been included in the treatment of the inert vapor in the modified RAILCAR tank algorithms. Reduced pressure leads lower jet mass flow rate. In terms of response to real-world incidents, though, this effect is minor.

With the modifications and additions resulting in RAILCAR3, the original entrainment factor of 0.2 for sheltered conditions led to good agreement with cloud durations observed from the videos. The range for this parameter to fit each trial ranged from 0.1 to more than one (1). The observed cloud durations are much shorter than the original RAILCAR predicts using the low volumetric air entrainment ratios, but the entrainment factor is appropriate when used with the much higher entrainment ratios. That value also predicts that the two (2) field trials

occurring under higher wind speeds do not lead to stationary cloud formation, consistent with observations.

2.5   Comparison with Jack Rabbit Data

The following RAILCAR input parameters were available and used during the pilot tests and field trials:

- Two (2)-m wind speed → average of anemometers around the pit
- Pit wind speed → single anemometer within the pit; used for liquid pool evaporation
- Two (2)-m air temperature → average of thermocouples around the pit
- Relative humidity
- Initial pressures in the vapor and liquid spaces → sensors inside tank at top and bottom; used to determine inert gas pressure
- Initial tank temperature → thermocouple inside tank at bottom

The following data were used to estimate atmospheric stability and friction velocity:

- Eight (8)-m wind speed → average of anemometers around the pit; used with two (2)-m wind speed to compute vertical wind speed gradient
- Eight (8)-m air temperature → average of thermocouples around the pit; used with two (2)-m air temperature to compute vertical air temperature gradient
- Ground temperature → average of four (4) thermocouples just below the surface within the pit; compared with two (2)-m air temperature

The following data and observations were used for comparison with RAILCAR output:

- Pressures in the vapor and liquid spaces versus time → sensors inside tank at top and bottom (available for all 10 tests/trials)
- Tank temperature versus time → thermocouple inside tank at bottom (available for all 10 tests/trials)
- Jet liquid and vapor durations → from video and tank pressure profiles (available for all 10 tests/trials)
- Cloud temperature → from thermocouples within the pit (available for eight (8) tests/trials)
- Cloud diameter and depth → estimated from video and 50-m pit diameter (available for five (5) tests/trials)
- Cloud duration → no visible persistent vapor within pit in video (available for seven (7) tests/trials)
- Liquid pool diameter → from video after cloud has dissipated and pit soil inspection (available for four (4) trials)
- Liquid pool duration → no visible vapor flux from pit surface near plate (available for six (6) tests/trials)

The author was not on-site to observe the last two (2) tests and had not received videos to estimate the cloud/plume and liquid pool behavior for comparison with RAILCAR3 predictions. Tank temperature, liquid space pressure, and vapor space pressure were recorded every 10 seconds until zero (0) gauge pressure was reached. In all cases, the pressures in the vapor and liquid spaces decreased together, with the difference only reflecting the liquid head pressure. The pressure in the vapor space was used for comparison with RAILCAR3 predictions. RAILCAR3 provides output at key transition points rather than at regular time intervals. The relevant RAILCAR3 output times are:

- Tank and jet properties at release time
- Tank and jet properties and time when depressurization begins
- Tank properties and time when the tank is empty
- Liquid pool properties when depressurization begins
- Time at which the liquid pool is gone
- Time at which liquid absorbed into the ground is gone
- Mist pool/stationary cloud properties when depressurization begins
- Time at which all aerosol has evaporated from a mist pool
- Time at which the mist pool/stationary cloud is gone

For comparison of predicted versus measured tank and jet properties, then, the starting pressure in the tank vapor space and temperature are RAILCAR3 input parameters, and the final pressure is set to ambient. The predicted values that can be compared are:

- Liquid jet duration (i.e., time when depressurization begins)
- Tank empty time (i.e., time when tank gauge pressure reaches zero (0))
- Pressure in the tank vapor space when depressurization begins
- Liquid temperature in the tank when depressurization begins
- Temperature at the tank empty time

Figures 6 and 7 show the predicted versus measured comparison for one (1) ammonia and one (1) chlorine field trial. The RAILCAR3 errors (predicted minus measured) for each trial for pressure in the tank vapor space when depressurization begins, liquid temperature in the tank when depressurization begins, temperature at the tank empty time, liquid jet duration, and tank empty time for all the tests and trials are included in Table 2. The RAILCAR3 errors for each trial for which data or observations are available for stationary cloud temperature, stationary cloud diameter, stationary cloud duration, liquid pool diameter, and liquid pool duration are included in Table 3. To get an idea of the magnitude of the errors, the average value of each property is:

- Pressure in the tank vapor space when depressurization begins = 4.42 atm
- Liquid temperature in the tank when depressurization begins = 4.2 °C
- Temperature at the tank empty time = -38.3 °C
- Liquid jet duration = 42 s
- Tank empty time = 77 s
- Stationary cloud temperature = -18 °C

- Stationary cloud diameter = 100 m
- Stationary cloud duration = 22 min
- Liquid pool diameter = 8 m
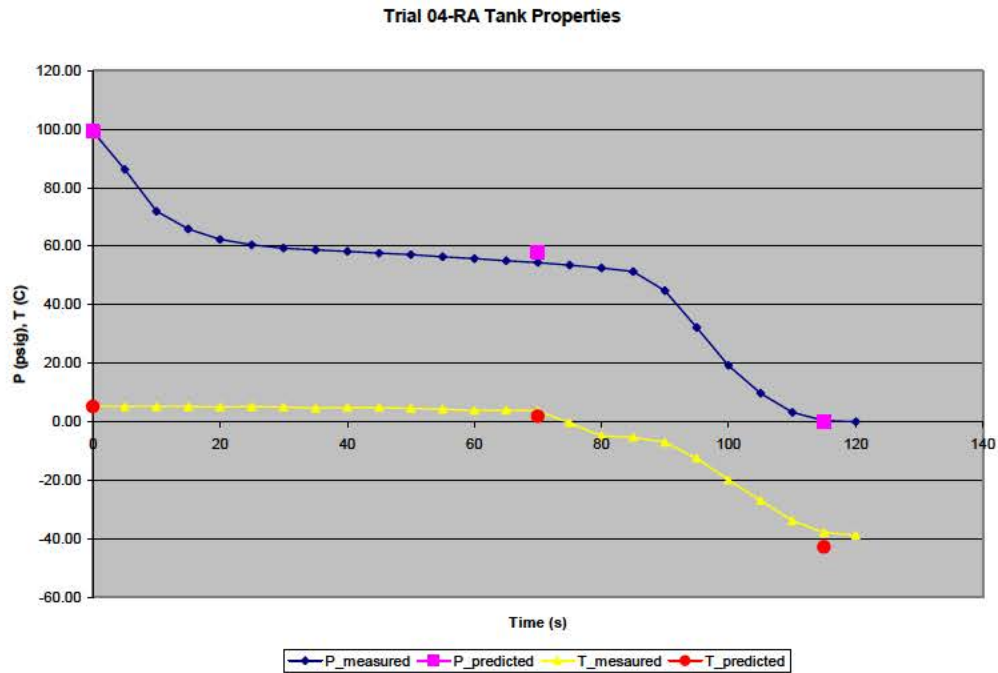- Liquid pool duration = 12 min (subsequent off-gassing averaged an additional 31 min)

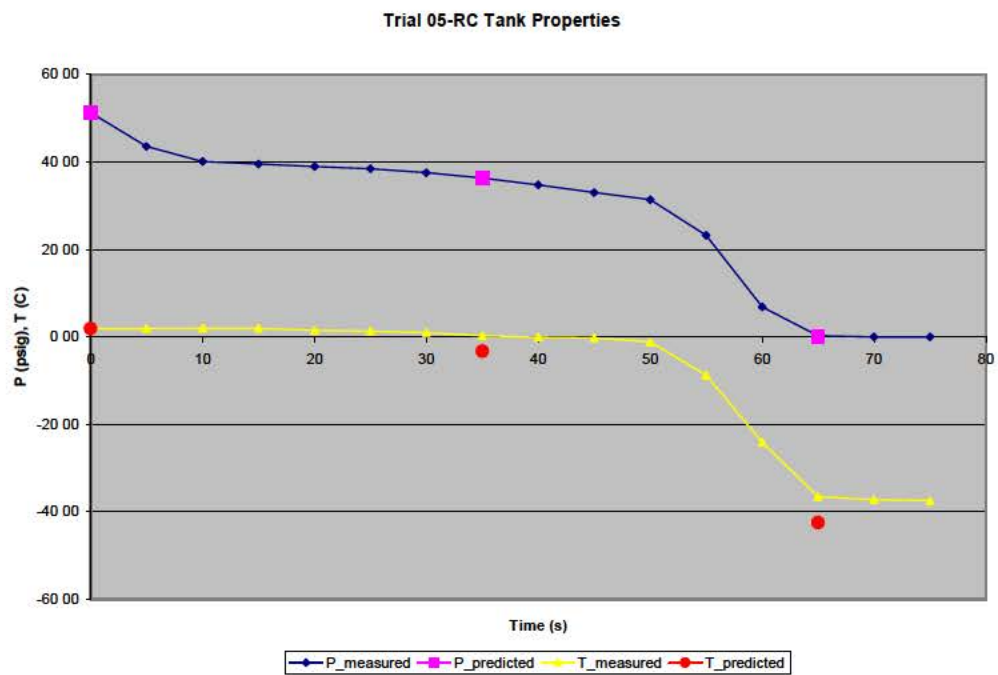Figure 6. Comparison of RAILCAR3 Predictions with Data for Ammonia Trial 04-RA

Figure 7. Comparison of RAILCAR3 Predictions with Data for Chlorine Trial 05-RC

Table 2. RAILCAR3 Prediction Errors for Tank and Jet Properties

Trial	ΔP (atm)	ΔT_d (C)	ΔT_f (C)	Δt_d (s)	Δt_f (s)
01-PA	0.38	-4.2	-3.2	3	-1
02-PC	0.25	-8.0	3.7	7	-2
03-RA	0.19	-1.5	-3.0	-1	3
04-RA	0.25	-1.8	-4.0	1	-3
05-RC	0.00	-3.6	-5.0	-1	1
06-RC	0.04	-3.4	-5.5	-4	0
07-RC	0.15	-3.1	-5.0	-5	0
08-RC	0.28	-3.4	-5.1	-10	3
09-RA	0.68	-2.1	-5.9	-1	-1
10-RA	0.85	-1.9	-7.9	-1	0
Avg.	0.31	-3.3	-4.1	-1.2	0

Table 3. RAILCAR3 Prediction Errors for Stationary Cloud and Liquid Pool Properties

Trial	ΔT_c (C)	Δd_c (m)	Δt_c (min)	Δd_p (m)	Δt_p (min)
01-PA	-4.4	-38	-16		9
02-PC	-10.2	7	11		
03-RA	1.3		3		-5
04-RA	1.4		6	0	8
05-RC	-0.5	11		0	
06-RC	NA	NA	NA	-1	0
07-RC	-3.0	3	-7	0	1
08-RC	-2.3		-16		-6
Avg.	-2.5	-4	-3	0	1

2.6 RAILCAR4 Development

The videos and processed data for the two (2) pilot tests and eight (8) record tests have since been provided to the test team. Some of the input parameters have been adjusted based on careful observation of the videos, and missing data has been extracted to provide an almost complete set of RAILCAR inputs and data to compare with RAILCAR output. A final calibration has been conducted where empirical parameters for:

- Rainout percent
- Foaming liquid percent
- Orifice vaporization percent
- Pool depth
- Liquid ground absorption percent

- Air entrainment ratio
- Cloud height
- Sheltering factor

have been adjusted for each test to match:

- Liquid empty time
- Tank empty time
- Cloud temperature
- Cloud diameter
- Cloud duration
- Pool diameter
- Pool evaporation duration
- Liquid off-gassing duration

The empirical input parameters were then averaged to provide the final set of recommended input values. For some of these parameters, the average values for ammonia and chlorine were significantly different, so recommended values are provided for ammonia, chlorine, and other chemicals.

In conducting the final calibration, enough modifications were made to the program to result in a new RAILCAR4. The pool evaporation methodology was changed to use ground temperature for evaporating liquid pools and the chemical boiling temperature for boiling liquid pools. The chemical properties at the appropriate temperature are now obtained within that subroutine. Ground temperature was added as an input parameter. A correction was made to the liquid jet pressure drop to correctly account for the orifice vaporization. The sheltering factor of five (5) was replaced by a user input to allow the cloud duration to be matched. Figures 8 and 9 show the fit and recommended temperature and pressure results with the RAILCAR3 results in Figures 6 and 7. The final prediction errors are displayed in Table 4.
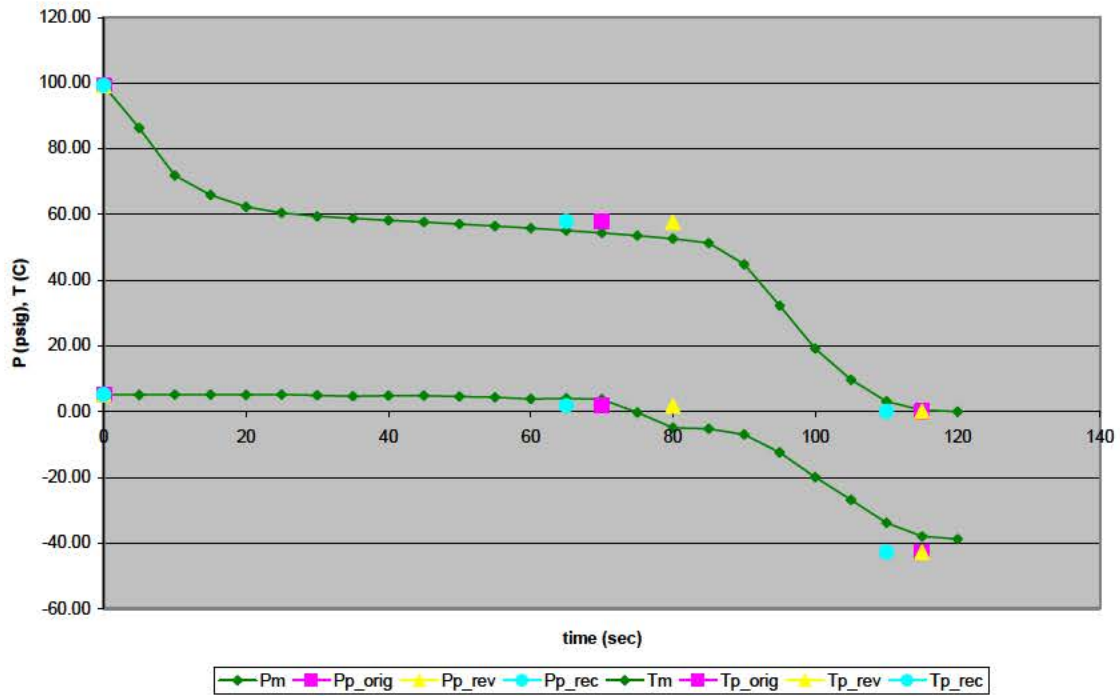
1 May Trial 04-RA

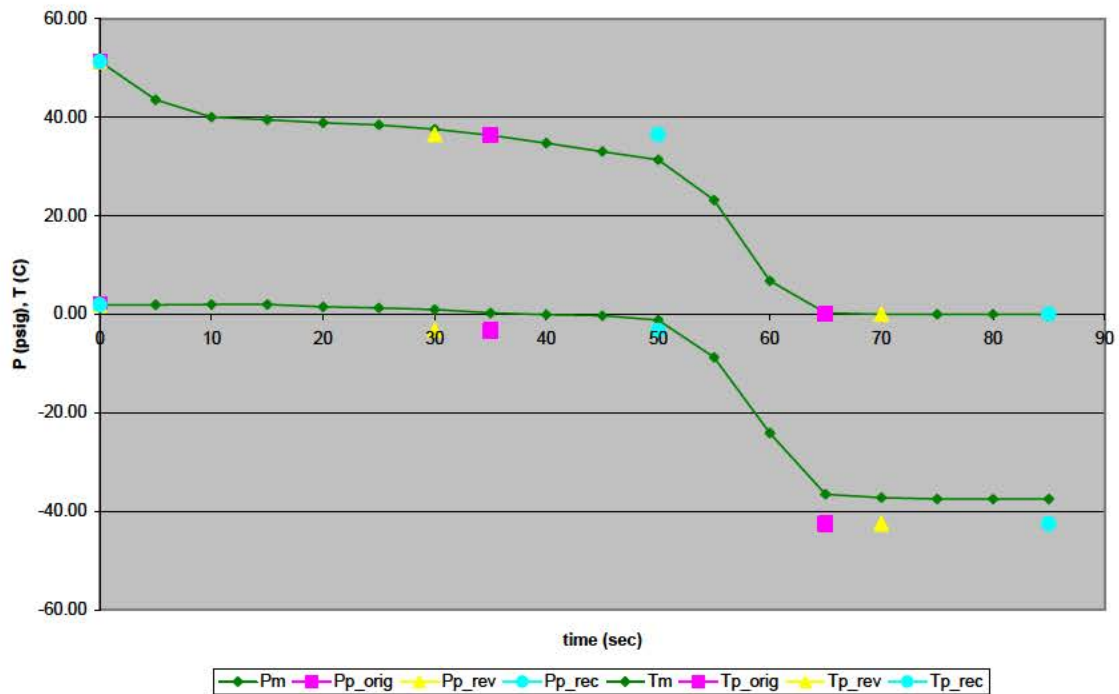Figure 8. RAILCAR4 Predictions for Ammonia Trial 04-RA

3 May Trial 05-RC

Figure 9. RAILCAR4 Predictions with Data for Chlorine Trial 05-RC

Table 4. RAILCAR4 Prediction Errors

absolute % error	7-Apr	8-Apr	27-Apr	1-May	3-May
chemical	ammonia	chlorine	ammonia	ammonia	chlorine
final temperature drop (°K)	7.8	7.4	6.0	8.6	12.4
depress. temp. drop (°K)	92.9	1200.0	18.2	70.0	333.3
depress. press. drop (atm)	17.6	13.8	6.7	8.7	4.1
liquid empty time (s)	11.8	2.3	26.0	21.0	56.3
tank empty time (s)	18.7	3.8	21.2	6.9	25.0
cloud temperature drop (°K)	61.5	53.8	29.6	3.7	7.8
cloud diameter (m)	49	22	26	17	17
cloud duration (min)	15	73	8	60	3
pool diameter (m)	30	50	10	18	12.5
pool duration (min)	180	150	40	1	8
off-gassing duration (min)	NA	NA	15	5	75

absolute % error	4-May	5-May	7-May	20-May	21-May	average
chemical	chlorine	chlorine	chlorine	ammonia	ammonia	
final temperature drop (°K)	13.1	10.8	13.2	10.9	16.5	10.7
depress. temp. drop (°K)	36.6	107.7	51.5	12.8	2.4	192.5
depress. press. drop (atm)	32.2	24.6	29.2	27.0	63.2	22.7
liquid empty time (s)	4.3	6.0	5.4	0.0	16.7	15.0
tank empty time (s)	30.6	17.6	20.5	6.1	13.8	16.4
cloud temperature drop (°K)	16.9	37.7	11.7	NA	NA	27.8
cloud diameter (m)	NA	0	5	68	NA	26
cloud duration (min)	NA	27	18	96	NA	38
pool diameter (m)	17	17	17	10	10	19
pool duration (min)	14	29	24	50	20	52
off-gassing duration (min)	36	10	10	22	50	28

3   RAILCAR4.1 OPERATOR'S INSTRUCTIONS

This section guides the operator in using the RAILCAR4.1 program. Some fairly minor additions have been made to the RAILCAR4 input parameters and output file. The major change is that a graphical user interface (GUI) has been added to RAILCAR4 to make parameter input much more user-friendly and to provide a clear visual representation of the predicted source characterization parameters. In addition, a second output file has been created which contains parameters required by an ATD model for characterizing the source predicted by RAILCAR. The current version has been designated RAILCAR4.1. The thermodynamic properties needed for each TIC are described to allow the user to update physical properties or add data for a TIC not currently addressed by the program. Operation of the GUI is described using an example run that simulates the Jack Rabbit ammonia pilot test. The input parameters are discussed along with the supporting algorithms, where applicable. Guidance is provided as to how best to interpret the output generated as inputs to ATD models for downwind toxic hazard area and concentration challenge level estimation.

3.1   TIC Thermodynamic Property File

Thermodynamic properties for each of the 49 chemicals addressed by RAILCAR4.1 have been extracted from reputable literature sources or estimated from accepted empirical relations.[28-35] The thermodynamic properties for each chemical are contained in a single file named RAILCAR.PAR. This approach allows the user to substitute more reliable or acceptable values when they are located or measured. The approach also allows the user to add additional chemicals to the file if the appropriate thermodynamic properties are available. The format for each chemical is identical, with entries being separated by one (1) or more spaces. RAILCAR4.1 is written in FORTRAN 77, with the numerical file entries read in free format. The records for each TIC in RAILCAR.PAR consist of six (6) lines:

Line	Parameter(s)
1	character string for the TIC name (25-character limit)
2	freezing temperature (°C)
	critical temperature (°C)
3	molecular weight (g/mole)
	liquid viscosity at 20 °C (cp)
	liquid heat capacity (specific heat) at boiling temperature (kJ/kg-K)
	vapor heat capacity (specific heat) at boiling temperature (kJ/kg-K)
	liquid surface tension at boiling temperature (dynes/cm)
	vapor diffusivity at 20 °C (cm^2/s)

4 liquid density at boiling temperature (kg/m^3)
   liquid density rate of change with temperature (kg/m^3-K)
5 Antoine constants A, B, and C for temperature in °C and pressure in atmospheres
6 heat of vaporization at boiling temperature (kJ/kg)
   heat of vaporization rate of change with temperature (kJ/kg-K)

The chemicals in the file are in alphabetical order. The records created for nitric acid are listed in Figure 10. Liquid viscosity is only used for the jet flow rate at the tank liquid temperature, so the value should not be significantly different than that at 20 °C. Vapor and liquid heat capacity values are adjusted for temperature within the program; the original mist pool methodology assumed the values are constant with temperature. Liquid surface tension is only used for aerosol formation during adiabatic expansion, which occurs at the TIC boiling temperature. Boiling temperature is computed from the Antoine constants for a pressure of one (1) atm. Vapor diffusivity is used for pool evaporation and is also adjusted for temperature within the program; pool evaporation is not addressed by the mist pool methodology.

```
nitric acid
-41.60  500.00
63.01   0.76     1.39     0.85  40.9  0.105
1332.9  -2.700
5.6270  2003.00  273.150
659.00  -0.952
```
Figure 10. Nitric Acid Thermodynamic Properties

Vapor pressure, liquid density, vapor density, and heat of vaporization are all relevant to multiple processes inside and outside of the tank, and a wide range of temperatures is relevant. Vapor density is computed from vapor pressure, temperature, and molecular weight using the ideal gas equation. These physical properties vary considerably with temperature. In general, the lowest temperature of interest is the greater of the freezing temperature and -100 °C for high-volatility chemicals and the higher of the freezing temperature and -20 °C for lower volatility chemicals. The highest temperature of interest is 50 °C, except in the case of chemicals that react and heat up when exposed to humid air or surface materials, such as sulfuric acid. The temperature range for sulfuric acid may extend to 200 °C. The temperature range of -20 °C to 50 °C is considered to cover the range of possible ambient temperatures, which usually also apply to the temperature of the liquid in the tank; however, refrigerated liquids like LNG and LPG will be at much lower temperatures. RAILCAR.PAR is located in the same directory as the RAILCAR4.1 executable.

3.2   RAILCAR4.1 Operation

The RAILCAR4.1 GUI has been written in Java and compiled for operation on a Microsoft Windows personal computer. Apple and UNIX/LINUX operating systems can also be supported. The RAILCAR4.1 executable is started by double-clicking on the executable icon labeled Railcar.jar. Input file RAILCALC.DAT is opened and contains the input parameter values from the last run. If RAILCALC.DAT doesn't exist in the executable directory, the default parameter values are used. The Tank Properties parameter input window is displayed in Figure 11 as set up to simulate the Jack Rabbit ammonia pilot test.

Figure 11. RAILCAR4.1 Tank Properties Input Window

All of the RAILCAR4.1 executable files must exist in the same directory as Railcar.jar, and the output files are generated in that same directory. The required executable files are:

- RAILCAR.PAR—chemical physical properties file previously described
- railcalc.exe—executable for performing the RAILCAR computations and generating the output summary file
- railcar.properties—properties file that specifies stand-alone of operation with an ATD model
- lib\beansbinding-1.2.1.jar—Java library file
- lib\commons-exec-1.1.jar—Java library file

The parameter input file (e.g., RAILCAR.DAT) is created after all parameters have been defined and the user executes the program; the user will be prompted for a file location and name. If the file already exists, it is overwritten with the new parameter values. An example parameter input file for the Jack Rabbit ammonia pilot test is provided in Figure 12.

```
ammonia
0     907.0000  0.0000
-0.10     0.7  -0.50      78.00      0      0.0000
          0
0.0000    0    0.0300    2.1300    0.6000    0.0600
0    0.4100
2    1    4.000    2.000      0.000      0.000
1    0.1500    0.0350    0.0000
0.0780    290.00    1.70
0.3000    0.0160    3    4.10
0.0000    5    0.0500    0    1000.0000  1
0.0  0.0
```

Figure 12. Example RAILCAR4.1 Parameter Input File

The order of the input parameters by line is:

- TIC name
- mass input type, initial tank mass, recovered liquid mass
- air temperature, ground temperature, tank temperature, relative humidity, terrain elevation type, surface height or pressure
- tank pressure, liquid head pressure mode, liquid head pressure, inert gas head pressure, ullage volume fraction, aerosol fraction rained out due to impaction
- tank thickness input type, tank thickness
- hole/pipe parameter type, orifice type, equivalent hole/pipe diameter, orifice diameter, hole area, orifice area

- liquid foaming flag, liquid mass fraction becoming foam, minimum vaporization mass fraction, pool mass fraction absorbing into ground
- liquid pool depth, entrainment ratio, cloud height
- wind speed at two (2) meters height, friction velocity, entrainment factor, sheltering factor
- wind speed at 10 meters height, surface type, surface roughness length, Pasquill stability category, Monin-Obukhov length, friction velocity flag
- release coordinates

Other than the first line containing the name of the TIC, the input files are free format separated by spaces or tabs. The input parameters are defined in the next section detailing operation of the parameter input window.

The user selects an existing file by clicking on the **Load Input File** button. The file navigation window displayed in Figure 13 appears, and the user navigates to the directory containing the desired RAILCAR4.1 input file and selects it in the usual Microsoft Windows fashion.
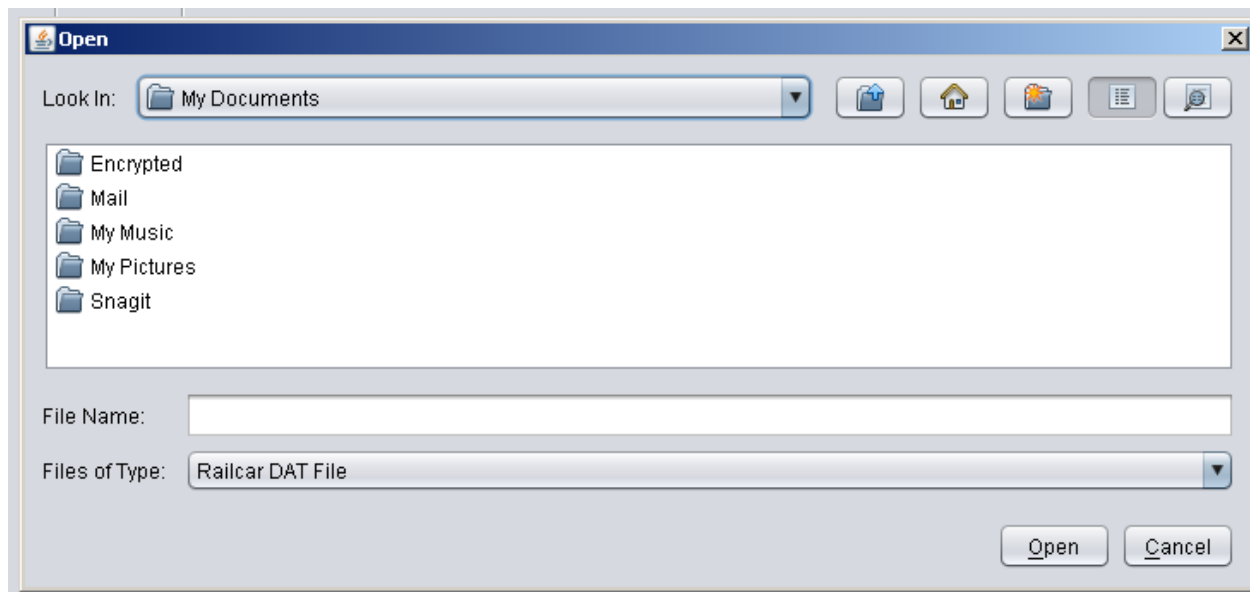
Figure 13. File Navigation Window

The GUI contains three (3) parameter input windows organized by parameter category: Tank Properties, Environmental Conditions, and Event Properties. The Tank Properties Input Window is displayed above in Figure 11. The Environmental Conditions Input Window is presented in Figure 14, and the Event Properties Input Window is presented in Figure 15. Once the input parameters have been defined and the user clicks on the **Run** button, Railcar.jar records the input parameters to the current input file and RAILCALC.DAT and executes railcalc.exe. Any changes made to the input parameters will be saved in the selected input file

unless the user saves a new file. Railcalc.exe expects the same input file name each time it runs, so RAILCALC.DAT is read rather than the file selected by the user.

Figure 14. Environmental Conditions Input Window

Figure 15. Event Properties Input Window

3.3 Input Parameters and Algorithms

RAILCAR4.1 has a total of 41 parameters used to define each incident. Several combinations of meteorology parameters can be entered by the user to determine the two (2)-m wind speed and friction velocity required by the program; the relation between the meteorology variables is addressed in Section 3.4. Parameters can be entered by the user or read from an existing input data file. Not all of the parameters are relevant to every run. Since it is difficult to determine prior to a simulation which processes are relevant and which are not, all values are displayed, with the parameters not relevant to an incident being assigned default values. The RAILCAR4.1 GUI provides a complete set of values upon start-up (default or from the previous

run), but the user is still responsible for ensuring that the set of parameters displayed is consistent with the incident being simulated. This section addresses the input parameters displayed in Figures 11, 14, and 15.

1. **Material**: The name of the TIC to be released in the simulation. The character string in the input file must match one (1) of the names in file RAILCAR.PAR. The user selects a TIC from the list in the pull-down menu displayed in Figure 16. The TIC for the Jack Rabbit pilot test for the example run is ammonia. Default = chlorine.
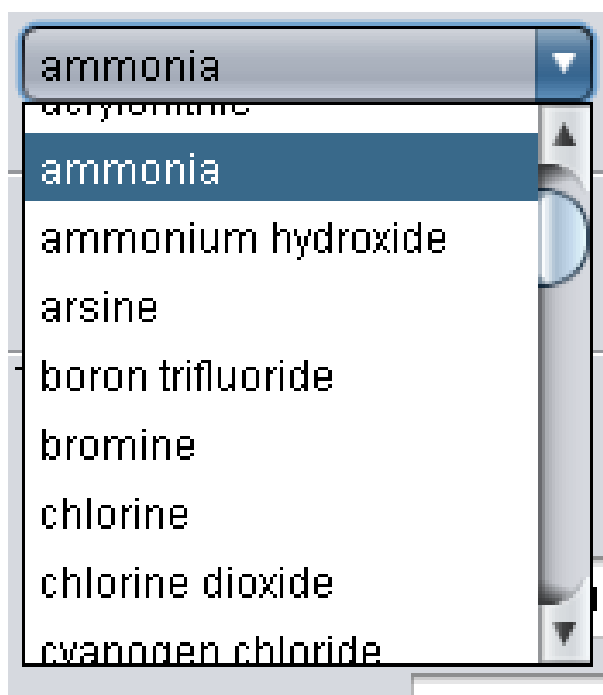
Figure 16. TIC Pull-Down Menu

2. **Mass Input Type**: The mode used to define the tank mass. The TIC masses in the tank and remaining after the tank is empty can be entered as either **Tank Mass** in kilograms or in terms of the chlorine **Tank Size** in U.S. tons. For example, chlorine Department of Transportation (DOT) 105A500W railcars are filled by weight to 90 tons chlorine liquid. If the user wishes to use the same railcar type with a different TIC, the user can enter 90 tons, and the program will calculate the correct fill mass using relative liquid densities. The units of measurement are U.S. tons equal to 2,000 pounds rather than metric tons equal to 1,000 kg. The liquid density of ammonia is 43.3% that of chlorine liquid, so the resulting ammonia fill mass will be (90 tons)(2,000 lb/ton)(1 kg/2.2046 lb)(0.433) = 35,353 kg. To select the Mass Input Type, the user clicks on one (1) of the radio buttons. The Mass Input Type for the Jack Rabbit ammonia pilot test is Tank Mass. Default = Tank Size.

3. **Initial Mass**: The mass in kilograms of TIC in the tank at the time of hole formation. The Initial Mass must be within the range of 100 kg (~0.1 U.S. ton) to 4E7 kg (~40,000 tons). If the Mass Input Type is chlorine Tank Size, the number of tons of chlorine for that tank type is entered. The number of tons must be within the range of 0.1 ton to 40,000 tons. The user enters the desired value and records it by pressing the Tab key or clicking on another parameter entry field. Initial Mass for the example run is 907 kg, which equals one (1) U.S. ton. Default = 90 tons.

4. **Remaining Mass**: The mass in kilograms of TIC liquid remaining in the tank after depressurization is complete. The range for Remaining Mass is from zero (0) kg to the Initial Mass in kilograms. If the Mass Input Type is chlorine Tank Size, the number of tons of chlorine that would remain for the tank type and hole position is entered, and the range for Remaining Mass is from zero (0) tons to the Initial Mass in tons. RAILCAR4.1 allows the hole to be generated in either the liquid space or the vapor space of the tank, except for TICs that exist only as vapor at the Tank Temperature (i.e., tank temperature is above the critical temperature). For holes generated in the liquid space, whether pressurized liquid or liquids below their boiling temperatures, the liquid will empty to the level of the bottom of the hole. Pressurized liquids will auto-refrigerate to their boiling temperatures within the tank during depressurization. The resulting vapor pressure is the same as the ambient pressure at the terrain elevation, so there will be no significant vapor flux out of the tank after that time. If the hole is generated in the vapor space for a pressurized liquid, the mass of liquid required to vaporize to cool the liquid to its boiling temperature at ambient pressure will be computed, and the remaining liquid mass will be adjusted. Liquids transported or stored below their boiling temperatures will already have a vapor pressure less than ambient pressure, so there will again be no significant vapor flux after the vapor-liquid interface reaches the bottom of the hole. There will be no tank depressurization for these liquids, and a hole in the vapor space will result in no mass leaving the tank. If one (1) of the five (5) representative hole types is selected for Hole/Pipe Parameter Type, the position of the hole will be specified. Remaining liquid mass will be determined from the Initial Mass and Ullage Volume Fraction. The hole in the Jack Rabbit tanks was at the tank bottom, so Remaining Mass is zero (0) kg. Default = 40 tons.

5. **Tank Temperature**: The temperature in °C of the liquid and vapor in the tank at the time of hole formation. There is no range limit for tank temperature, which allows for contents to be heated or refrigerated. For liquid pools that heat up due to reaction with surface materials or humid air (e.g., sulfuric acid), the entered tank temperature should represent the temperature of the pool after heating. Tank temperature is expected to be within the range of validity for the thermodynamic property equations. Tank Temperature for the example run is -0.5°C. Default = 25°C.

6. **Tank Pressure**: The initial pressure in atmospheres (atm) inside the tank if the Tank Temperature exceeds the TIC critical temperature and there is no liquid phase in the tank. Tank Pressure must be greater than or equal to zero (0) atm. The Tank

Temperature for the example run is well below the ammonia critical temperature, so the default Tank Pressure of zero (0) atm is used. Default = Zero (0) atm.

7. **Default Tank Thickness**: Flag used to specify that the Tank Thickness is not known and that RAILCAR4.1 should calculate it. The Default Tank Thickness is based on the combined thickness of 4.897 inches for the tank, insulation, and jacket for a DOT 105A500W railcar and 0.50 inches for a one (1)-ton chlorine tank. The larger thickness is assumed for any tank containing more than 5,000 kg of liquid chemical. This parameter allows the user to define the tank thickness in place of these assumed values and is to be used to define the length of a pipe attached to the tank, such as when the incident involves a pipe break. The user activates the flag by clicking on the check box. Tank Thickness for the example run is known, so the Default Tank Thickness check box is left empty. Default = Selected.

8. **Tank Thickness**: The thickness in meters of the tank from the liquid inside to the air interface if the Default Tank Thickness check box is empty. Tank Thickness must be greater than or equal to zero (0) meters. If the incident involves a break in a pipe attached to the tank or failure of a valve at the end of a pipe, this parameter represents the length of pipe between the liquid inside and the location of the break or valve. RAILCAR4.1 combines the Bernoulli equation with frictional losses through the thickness of the tank or length of pipe. Based on observations during the Jack Rabbit pilot tests and field trials, there will be some vaporization before the hole opening if there is a pipe attached to a tank containing pressurized liquid. The Jack Rabbit tanks used a valve to remotely simulate a tank rupture. For safety reasons, a check valve was used in between the tank and the release valve. The combined fittings, valves, and pipe resulted in significant addition to the tank thickness. Effective Tank Thickness for the tank used for the example ammonia release is 0.41 meters. Default = Zero (0) meters.

9. **Ullage Volume Fraction**: The fraction of tank volume not occupied by liquid. This space will contain TIC vapor and any added or trapped inert vapor. The TIC vapor is assumed to be at equilibrium with the liquid, so the TIC vapor mass is determined by the vapor pressure at the Tank Temperature. The range for this value is from zero (0) to 0.75; the depressurization methodology diverges above 0.75. The typical Ullage Volume Fraction recommended by RAILCAR4.1 is 0.1 if the user does not know the correct value. This parameter is not used if the Tank Temperature exceeds the TIC critical temperature, as the all-vapor TIC will fill the entire tank. Ullage Volume Fraction for the Jack Rabbit ammonia pilot test is 0.6. Default = 0.1.

10. **Calculate Tank Pressure**: Flag used to specify that the initial Liquid Head Pressure in the tank is not known and that RAILCAR4.1 should calculate it. The aspect ratio of the DOT 105A500W is used to scale the tank volume to the appropriate tank diameter for the specified Initial Mass and Ullage Volume Fraction. The angles to the initial and final vapor-liquid interfaces are determined, which are then converted to Liquid Head Pressure in atm. This calculation is appropriate for most horizontal tanks such as those

on railcars and transport trucks. The user activates the flag by clicking on the check box. Liquid Head Pressure for the example run is known, so the Calculate Tank Pressure check box is left empty. Default = Selected.

11. **Liquid Head Pressure**: The pressure in atm at the bottom of the tank due to the height of liquid within the tank when the Calculate Tank Pressure check box is empty. Liquid Head Pressure must be greater than or equal to zero (0) atm. Liquid head pressure, P_{head}, follows the equation:

$$P_{head} = \rho_L\, g\, H_L/(101325\ Pa/atm) \hspace{3cm} [4]$$

where ρ_L is the liquid density in kg/m^3, and H_L is the liquid height in meters between the initial and final vapor-liquid interfaces. Liquid Head Pressure for the example run is 0.03 atm. Default = Zero (0) atm.

12. **Inert Gas Pressure**: The pressure in atm of nitrogen, air, or any inert gas added or trapped in the ullage space. Inert Gas Pressure must be greater than or equal to zero (0) atm. RAILCAR4.1 uses the thermodynamic properties of dry air for the gas, regardless of composition. Since air is 79% nitrogen, there is little error in using air properties for this most commonly added gas. If any gas other than nitrogen or air is added, the thermodynamic properties may be significantly different. This parameter is not used if the Tank Temperature exceeds the TIC critical temperature, as there is no reason to have other than the all-vapor TIC inside the tank at the entered Tank Pressure. Nitrogen in the amount of 2.13 atm was added to the Jack Rabbit ammonia pilot test in an attempt to prevent ammonia vaporization within the release valve configuration. Default = Zero (0) atm.

13. **Surface Type**: The type of ground surface over which the tank is located at the time of the incident. The user selects a surface from the list in the pull-down menu displayed in Figure 17. This entry is initially grayed out, based on the two (2)-m Wind Speed and Friction Velocity entries being activated. If the user does not know one (1) or the other of those parameters, and the Surface Type and other required alternate parameters are known, the user can activate the Surface Type by clicking on it. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. The two (2)-m Wind Speed and Friction Velocity are known for the example run, so the Surface Type entry remains grayed out. Default = grass.

14. **Roughness Length**: The effective height in meters of the ground surface components (e.g., grass, brush, buildings) over which the tank is located at the time of the incident. The range for Roughness Length is 0.0001 meter to one (1) meter. This entry is initially grayed out, based on the two (2)-m Wind Speed and Friction Velocity entries being activated. If the user does not know one (1) or the other of those parameters, and the Roughness Length and other required alternate parameters are known, the user can

activate the Roughness Length by clicking on it and entering a value. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. Note that the Roughness Length is typically 1/10th the average ground surface component height; entering the average height will lead to inappropriate meteorology conditions. The two (2)-m Wind Speed and Friction Velocity are known for the example run, so the Roughness Length entry remains grayed out. Default = 0.05 meters.
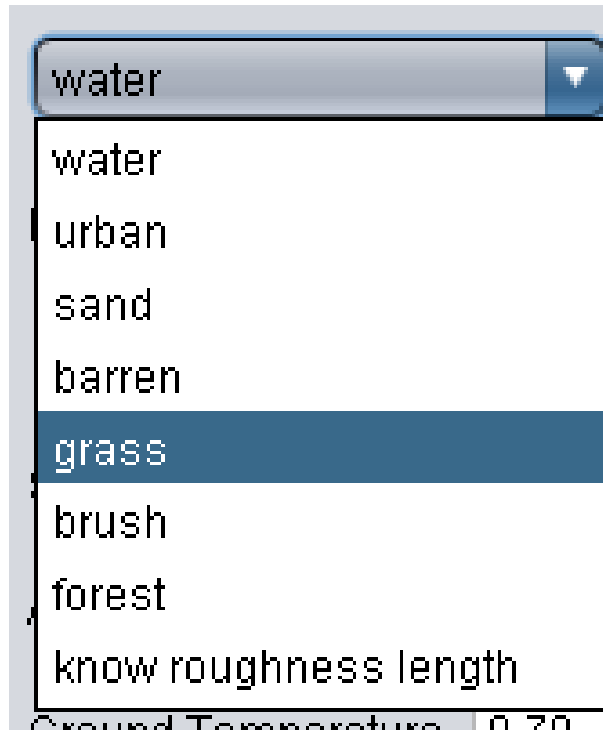
Figure 17. Surface Type Pull-Down Menu

15. **Entrainment Factor**: A rough characterization of the interaction of the jet with passing air. It is used to determine if the mist pool or stationary vapor cloud formation criterion is met and to calculate the mist pool/stationary cloud behavior if it is. The user selects a description from the list in the pull-down menu displayed in Figure 18. An Entrainment Factor of "enhanced" is appropriate if entrainment of the jet into the passing air is enhanced by the jet aiming upwards or with the wind or the terrain is flat and smooth; the mist pool algorithms then multiply the vapor flux by the Sheltering Factor. An entrainment factor of "sheltered" is appropriate if entrainment is inhibited by the presence of buildings, vegetation, and/or terrain undulations at the release location that shelter the jet from the ambient wind; the mist pool algorithms then divide the vapor flux by the Sheltering Factor. An entrainment factor of "normal" is appropriate if entrainment is neither enhanced nor sheltered, and a factor of one (1) is used in the

mist pool algorithms. The Jack Rabbit ammonia field trial used a two (2)-m deep pit to break up the linear airflow, so "sheltered" is selected. Default = normal.

Figure 18. Entrainment Factor Pull-Down Menu

16. **Sheltering Factor**: The value which the air entrainment ratio is multiplied by if the Entrainment Factor is "enhanced" and divided by if the Entrainment Factor is "sheltered". Sheltering Factor must be greater than one (1). This value is not used if the Entrainment Factor is "normal". The recommended value is 1.5 for ammonia, 4.5 for chlorine, and 3.0 for other chemicals. The Sheltering Factor for the example run resulting from RAILCAR4.1 Jack Rabbit calibration is 4.1. Default = 4.5.

17. **Air Temperature**: The temperature in °C of the ambient air at the time of hole formation. Air Temperature must be within the range of -15°C to 50°C, which is considered appropriate for relevant geographic locations. Air temperature is used for determining cloud equilibrium after air entrainment. RAILCAR4.1 does not allow for changes in meteorological conditions. If a mist pool or stationary cloud forms, vapor detrains into the passing air rather than air being entrained into the mist pool, so a change in air temperature will not affect the behavior of the mist pool/stationary cloud. Since meteorological conditions can be reasonably assumed to be constant for up to one (1) hour, this RAILCAR4.1 restriction is only a limitation if the release duration or pool evaporation duration exceeds one (1) hour. The Air Temperature for the example run is -0.1°C. Default = 25°C.

18. **Ground Temperature**: The temperature in °C of the ground at the time of hole formation. Ground temperature must be within the range of -15°C to 50°C, which is considered appropriate for relevant geographic locations. Ground temperature is used for computing the liquid pool evaporation rate and is assumed to be constant for the duration of pool evaporation. The Ground Temperature for the example run is 0.7°C. Default = 25°C.

19. **Relative Humidity**: The relative humidity in percent of the ambient air. Relative Humidity must be within the range of 0% to 100%. Relative Humidity is used to determine air density and contributes to cloud equilibrium by cooling, condensing, and freezing. RAILCAR4.1 does not allow for changes in meteorological conditions. Since meteorological conditions can be reasonably assumed to be constant for up to one (1) hour, this RAILCAR4.1 restriction is only a limitation if the release duration exceeds one (1) hour. The Relative Humidity for the example run is 78%. Default = 30%.

20. **Two (2)-m Wind Speed**: The surface wind speed in meters per second at the release location measured two (2) meters above the ground surface. Two (2)-m Wind speed must be greater than or equal to zero (0) m/s. The two (2)-m Wind Speed and Friction Velocity are required parameters for program execution and are initially activated. If the two (2)-m Wind Speed is not known for user input, it can be estimated from other parameters, which include 10-m Wind Speed, Friction Velocity, Surface Type, and atmospheric Stability Category. If the user knows the 10-m Wind Speed, they can activate the 10-m Wind Speed by clicking on it and entering a value; the two (2)-m Wind Speed will be grayed out. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. This parameter is only used for the liquid pool evaporation calculations. For the Jack Rabbit pilot tests and field trials, the appropriate wind speed was taken by the anemometer in the pit. RAILCAR4.1 does not allow for changes in meteorological conditions. Since meteorological conditions can be reasonably assumed to be constant for up to one (1) hour, this RAILCAR4.1 restriction is only a limitation if the pool evaporation duration exceeds one (1) hour. The two (2)-m Wind Speed for the example run is known and is 0.3 m/s. Default = Two (2) m/s.

21. **10-m Wind Speed**: The surface wind speed in meters per second at the release location measured 10 meters above the ground surface. Ten (10)-m Wind Speed must be greater than or equal to zero (0) m/s. The two (2)-m Wind Speed and Friction Velocity are required parameters for program execution and are initially activated. If the two (2)-m Wind Speed is not known for user input, it can be estimated from other parameters, which include 10-m Wind Speed, Friction Velocity, Surface Type, and atmospheric Stability Category. If the user knows the 10-m Wind Speed, they can activate the 10-m Wind Speed by clicking on it and entering a value; the two (2)-m Wind Speed will be grayed out. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. The two (2)-m Wind Speed for the example run is known, so the 10-m Wind Speed entry remains grayed out. Default = Zero (0) m/s.

22. **Friction Velocity**: The friction velocity in meters per second for the level of turbulence in the surface winds due to surface heating or cooling and interaction with the roughness elements of the ground surface. This parameter must be greater than zero (0) m/s. The two (2)-m Wind Speed and Friction Velocity are required parameters for program execution and are initially activated. If the Friction Velocity is not known

for user input, it can be estimated from other parameters, which include two (2)-m Wind Speed, 10-m Wind Speed, Surface Type, and atmospheric Stability Category. If the user knows the atmospheric Stability Category, they can activate the Stability Category by clicking on it and selecting an entry from the pull-down menu; the Friction Velocity will be grayed out. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. Friction Velocity is used to determine if a mist pool or stationary vapor cloud will form and to determine the resulting behavior if one does. For the Jack Rabbit pilot tests and field trials, the appropriate wind speed used to determine the friction velocity was taken by the anemometers just outside of the pit. RAILCAR4.1 does not allow for changes in meteorological conditions. Since meteorological conditions can be reasonably assumed to be constant for up to one (1) hour, this RAILCAR4.1 restriction is only a limitation if the release duration exceeds one (1) hour. The Friction Velocity for the example run is known and is 0.016 m/s. Default = 0.217 m/s.

23. **Stability Category**: Used to compute the Monin-Obukhov length, which characterizes the depth in meters of the surface layer turbulence. The user selects a category from the list in the pull-down menu displayed in Figure 19. This entry is initially grayed out, based on the two (2)-m Wind Speed and Friction Velocity entries being activated. If the user does not know one (1) of the other of those parameters, and the Stability Category and other required alternate parameters are known, the user can activate the Stability Category by clicking on it; the Friction Velocity will be grayed out. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. The two (2)-m Wind Speed and Friction Velocity are known for the example run, so the Stability Category entry remains grayed out. Default = neutral.
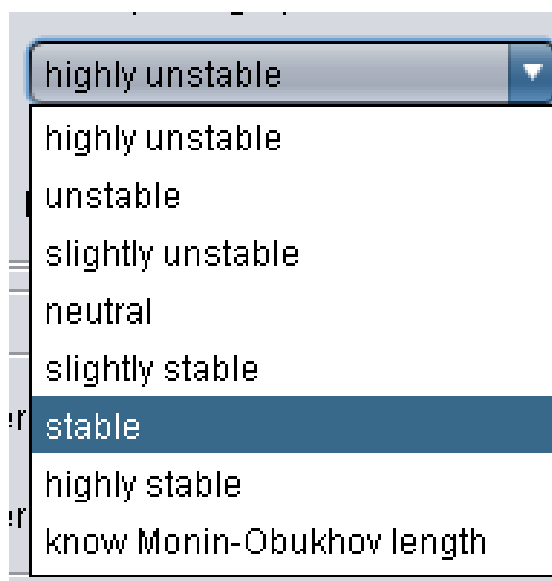

Figure 19. Atmospheric Stability Category Pull-Down Menu

24. **Monin-Obukhov Length**: Characterizes the depth in meters of the surface layer turbulence. This entry is initially grayed out, based on the two (2)-m Wind Speed and Friction Velocity entries being activated. If the user does not know one (1) of the other of those parameters, and the Monin-Obukhov Length and other required alternate parameters are known, the user can activate the Monin-Obukhov Length by clicking on it and entering a value. The parameter combinations that can be entered by the user to have RAILCAR4.1 determine two (2)-m Wind Speed and Friction Velocity are described in Section 3.4. The two (2)-m Wind Speed and Friction Velocity are known for the example run, so the Monin-Obukhov Length entry remains grayed out. Default = 1,000 meters.

25. **Terrain Elevation:** The mode used to specify the height of the ground surface above sea level. Elevated terrain decreases both ambient pressure and liquid boiling temperature. The height of the terrain can be defined in terms of **Surface Height** in meters or **Surface Pressure** in atmospheres. To select the Terrain Elevation mode, the user clicks on one (1) of the radio buttons. The height of the terrain for the example run is defined in terms of Surface Height. Default = Surface Height.

26. **Surface Height**: The height above sea level in meters at the release location. Surface Height must be greater than or equal to zero (0) meters. The ambient pressure is adjusted for the terrain elevation. The resulting lower ambient pressure leads to a lower boiling temperature and can affect a variety of other physical processes simulated by the program. A Surface Height of zero (0) meters is recommended for studies or where a specific release location and its associated height are not known. The Surface Height for the example run is set to zero (0) meters, as this parameter was not used for the Jack Rabbit calibration effort. The correct Surface Height at the test location is 1,306 meters. Default = Zero (0) meters.

27. **Surface Pressure**: The ambient pressure in atm at the release location. Surface Pressure must be less than or equal to one (1) atm. Surface Pressure should only be selected for a measured value or when using a correct correlation between pressure and height. An ambient pressure less than one (1) atm (signifying elevated terrain) leads to a lower boiling temperature and can affect a variety of other physical processes simulated by the program. The surface pressure at 1,306 m at the -0.1°C air temperature for the example run is 0.847 atm. Default = one (1) atm.

28. **Hole/Pipe Parameter Type**: The mode used to define the size of the hole and orifice through which the tank empties or to define both the hole size and angular location based on representative hole types. The size of the hole and orifice can be defined in terms of Diameter in inches or Area in square meters. Alternatively, the user can select from five (5) representative hole types designed to provide a range of realistic hole properties. Selecting one (1) of these hole types results in the hole diameter or area

and the angle to the hole being specified; the liquid Remaining Mass will then be determined by the Initial Mass and the Ullage Volume Fraction. The user selects a mode from the list in the pull-down menu displayed in Figure 20. The hole and orifice sizes for the example run are defined in terms of Diameter. Default = Diameter.
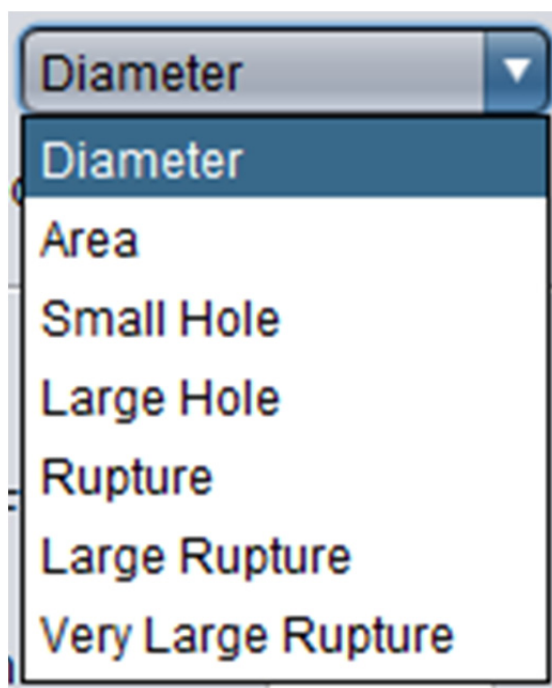
Figure 20. Hole/Pipe Parameter Type Pull-Down Menu

29. **Hole/Pipe Diameter**: The equivalent diameter in inches of the inner surface of the hole or pipe if the Hole/Pipe Parameter Type of Diameter is selected. Hole/Pipe Diameter must be greater than or equal to 0.2 inches. The inner diameter is assumed to be uniform through the thickness of the hole or length of the pipe up to the orifice if there is one. The jet flow methodology cannot be expected to be accurate for holes larger than about 12 inches in diameter; however, the tank empty time will be very short for such a large hole. This parameter is not displayed if the Hole/Pipe Parameter Type of Area or one (1) of the five (5) representative hole types is selected. The Hole/Pipe Diameter for the example run is 4.0 inches. Default = 3.0 inches.

30. **Hole/Pipe Area**: The inner area of the hole or pipe in square meters if the Hole/Pipe Parameter Type of Area is selected. Hole/Pipe Area must be greater than or equal to 2E-5 m^2. The inner diameter is assumed to be uniform through the thickness of the hole or length of the pipe up to the orifice if there is one. The jet flow methodology cannot be expected to be accurate for holes larger than about 0.07 m^2 (12 inches in diameter); however, the tank empty time will be very short for such a large hole. This parameter is not displayed if the Hole/Pipe Parameter Type of Diameter or one (1) of

the five (5) representative hole types is selected. The hole size for the example run is defined in terms of Diameter, so this parameter is not displayed. Default = 4.6E-3 m^2.

31. **Orifice Type**: The mode used to define whether there is a decrease in hole size at the orifice location. An orifice can be placed at the air interface of the hole or pipe to restrict flow, as designed for the Jack Rabbit pilot tests and field trials. RAILCAR4.1 assumes the transition between the hole or pipe and the orifice is smooth and does not add additional frictional losses other than due to the reduced area. If the hole size is reduced at the orifice, the orifice is **Restricted**; otherwise, the orifice is **Unrestricted**. This parameter is not used if one (1) of the five (5) representative hole types is selected for Hole/Pipe Parameter Type. To select the Orifice Type, the user clicks on one (1) of the radio buttons. A restricting orifice was used for the Jack Rabbit ammonia pilot test to try to prevent vaporization within the pipe, so the Restricted radio button is selected. Default = Unrestricted.

32. **Orifice Diameter**: The diameter in inches of the inner surface of the orifice positioned at the air interface of the hole or pipe if the Hole/Pipe Parameter Type of Diameter is selected. Although there is no check within RAILCAR4.1, the Orifice Diameter must be smaller than the Hole/Pipe Diameter. If the Orifice Type of Unrestricted is selected, the Orifice Diameter is set equal to the Hole/Pipe Diameter and is grayed out. This parameter is not displayed if the Hole/Pipe Parameter Type of Area or one (1) of the five (5) representative hole types is selected. The orifice Diameter for the example run is 2.0 inches. Default = 3.0 inches.

33. **Orifice Area**: The inner area in square meters of the orifice positioned at the air interface of the hole or pipe if the Hole/Pipe Parameter Type of Area is selected. Although there is no check within RAILCAR4.1, the Orifice Area must be smaller than the Hole/Pipe Area. If the Orifice Type of Unrestricted is selected, the Orifice Area is set equal to the Hole/Pipe area and is grayed out. This parameter is not displayed if the Hole/Pipe Parameter Type of Diameter or one (1) of the five (5) representative hole types is selected. The orifice size for the example run is defined in terms of Diameter, so this parameter is not displayed. Default = 4.6E-3 m^2.

34. **Aerosol Fraction Rained Out**: The fraction of liquid mass in aerosol form following adiabatic expansion of the jet which impacts the ground surface and forms a liquid pool. The range for this value is from zero (0) to one (1). This parameter is reset to one (1) if the Tank Temperature is below the TIC boiling temperature, as the jet will be all liquid with all of the mass depositing onto the ground surface. Similarly, RAILCAR4.1 assumes that a Tank Temperature less than 20°C above the boiling temperature (i.e., liquid superheat) generates large droplets that also deposit onto the ground surface and resets the rainout fraction to one (1). The rainout fraction recommended by RAILCAR4.1 is 0.1 for ammonia, 0.5 for chlorine, and 0.3 for other chemicals if the jet is aimed downward and zero (0) otherwise. The jet will be aimed downward if the hole is below

the midpoint of the tank. The Aerosol Fraction Rained Out for the example run is 0.06. Default = Zero (0).

35. **Foaming Occurs**: Flag used to specify that the liquid in the tank foams when the hole/rupture occurs. The extended depressurization time for Jack Rabbit pilot tests and field trials showed that the near-instantaneous pressure drop at the hole leads to foaming of the pressurized liquid within the tank ullage volume. The user activates the flag by clicking on the check box, which is recommended for releases of pressurized liquid. Foaming is not relevant to chemicals stored as all-vapor or chemicals stored at temperatures below the boiling temperature. Foaming did occur for the example run, so the check box is selected. Default = Selected.

36. **Liquid Fraction Becoming Foam**: The fraction of initial liquid that becomes foam mixed with the initial vapor in the ullage volume. The range of this parameter is from zero (0) to one (1). Based on the Jack Rabbit data, a value of 0.065 is recommended for pressurized liquids. The Liquid Fraction Becoming Foam determined for the example run is 0.15. Default = 0.065.

37. **Minimum Vaporization Fraction**: The fraction of liquid in the pipe that vaporizes prior to the air interface. The range of this parameter is from zero (0) to one (1). The slower liquid flow rate and shape of the jet during the Jack Rabbit pilot tests and field trials suggest that vaporization occurs if a pipe is attached to the tank. The recommended value for pressurized liquids is 0.035 if flow is through a pipe and zero (0) otherwise. The Minimum Vaporization Fraction determined for the example run is 0.035. Default = Zero (0).

38. **Liquid Pool Depth**: The depth or thickness in centimeters of the boiling or evaporating liquid pool formed from rainout from the jet. Liquid Pool Depth must be greater than or equal to zero (0) centimeters. Observations of liquid pools on fairly smooth surfaces suggest the pool depth will not exceed one (1) centimeter. Pool depth is expected to be thicker on rough surfaces. Liquid pool formation is expected for chemicals stored at temperatures below the boiling temperature, chemicals stored at temperatures less than 20°C above the boiling temperature, and chemicals stored at higher superheat where the jet impacts the ground surface. RAILCAR4.1 assumes that all liquid in the jet rains out for the first two cases and uses the aerosol fraction rained out due to impaction for the last case. A liquid pool will not form for chemicals stored as all-vapor. The recommended value is 0.3 centimeters for ammonia, 1.2 centimeters for chlorine, and 0.8 centimeters for other chemicals. The Liquid Pool Depth for the example run is 0.078 centimeters. Default = 1.2 centimeters.

39. **Pool Mass Fraction Absorbing Into Ground**: The fraction of mass in the boiling or evaporating liquid pool that absorbs into the porous ground surface and off-gasses at a rate slower than pool evaporation after the liquid mass on the surface is gone. The range of this parameter is from zero (0) to one (1). The ground surface in the pit

progressively degraded with each pilot test and field trial due to the interaction of ammonia, chlorine, and ice with the soil around the tank. The field trials had visible vapor off-gassing well after the liquid sitting on the surface had evaporated. Although repeated incidents at the same location are not expected, a value of 0.25 is recommended if the surface is porous and zero (0) otherwise. The Pool Mass Fraction Absorbing Into Ground for the example run is zero (0). Default = Zero (0).

40. **Entrainment Ratio**: The volume of air mixed into the jet over the volume of the jet. This parameter must be greater than or equal to zero (0). This parameter is used to determine if the mist pool or stationary vapor cloud formation criterion is met and to calculate the mist pool/stationary cloud behavior if it is. The recommended value, based on the Jack Rabbit data, is 180. A mist pool or stationary vapor cloud will not form for chemicals stored at temperatures below the boiling temperature. A stationary vapor cloud may form for chemicals stored as all-vapor due to formation of a very cold cloud upon expansion to ambient pressure. The Entrainment Ratio for the example run is 290. Default = 180.

41. **Cloud Height**: The height or thickness in meters of the mist pool or stationary vapor cloud after formation. This parameter must be greater than zero (0) meters. Like the Entrainment Ratio, this parameter is used to determine if the mist pool or stationary vapor cloud formation criterion is met and to calculate the mist pool/stationary cloud behavior if it is. The recommended value is four (4) meters. A mist pool or stationary vapor cloud will not form for chemicals stored at temperatures below the boiling temperature. A stationary vapor cloud may form for chemicals stored as all-vapor due to formation of a very cold cloud upon expansion to ambient pressure. The Cloud Height for the example run is 1.7 meters. Default = Four (4) meters.

3.4   Wind Condition Input

The wind speed at two (2)-m height and friction velocity at the release location are required inputs. These parameters are recorded to the input file. If the user does not know either of these values, the user can enter alternate parameters that are used to estimate them. There are four (4) combinations of meteorology parameters that can be used, the first of which is the two (2)-m wind speed and friction velocity, both in meters per second.

The second option is relevant if the friction velocity is known, but the wind speed measurement height is 10 meters instead of two (2) meters. In order to determine the two (2)-m wind speed, the surface type is needed. The surface type is used to compute the surface roughness length in meters. The user must enter the friction velocity and 10-m wind speed, both in meters per second. There are eight available surface types (see Figure 17):

- Water
- Urban
- Sand
- Barren
- Grass
- Brush
- Forest
- Know roughness length

The surface types are listed in order of increasing surface roughness length, which ranges from 0.001 meters to 0.4 meters. Alternately, the user may enter the value in meters if known.

The third option is relevant if the two (2)-m wind speed is known, but the friction velocity is not. In order to determine the friction velocity, the surface type and the Pasquill stability category are needed. The surface type is used to compute the surface roughness length in meters, and the Pasquill stability category is used to compute the Monin-Obukhov length, which characterizes the depth in meters of the surface layer turbulence. The user first enters the two (2)-m wind speed in meters per second. There are eight (8) available stability categories (see Figure 19):

- Highly unstable
- Unstable
- Slightly unstable
- Neutral
- Slightly stable
- Stable
- Highly stable
- Know Monin-Obukhov length

The last selection allows the user to enter the value for the Monin-Obukhov length in meters. Monin-Obukhov length is negative for unstable conditions, positive for stable conditions, and very large for neutral conditions.

The fourth option is relevant if the 10-m wind speed is known and the friction velocity is not. In order to determine the two (2)-m wind speed and friction velocity, the surface type and the Pasquill stability category are needed. The surface type is used to compute the surface roughness length in meters, and the Pasquill stability category is used to compute the Monin-Obukhov length in meters. The user enters the 10-m wind speed in meters per second, surface type, and Pasquill stability category.

3.5   Program Output

If the user defines a new incident using the input parameter window and selects Run, RAILCAR4.1 prompts the user to save the input parameters to a file. The File Navigation Window in Figure 13 is displayed with the word "Save" in place of "Open". The format of the file is as shown in Figure 12. The input parameters and a summary of calculated parameters are written to the output summary file, RAILCAR.OUT. The content of this file is addressed in Section 3.6. Parameters needed by hazard prediction models to define the source are written to a separate output file named RAILCALC.OUT. This file contains five (5) lines and includes the following values:

- Source type, final pool/cloud diameter (m), pool/cloud growth duration (s), pool/cloud final duration (s), vapor mass rate (kg/s)
- Cloud density (kg/m^3), cloud concentration (kg/m^3), cloud height (m), cloud vapor density (kg/m^3), cloud vapor concentration (kg/m^3)
- Droplet diameter (m), vapor temperature (°K), cloud vapor mass rate (Q_c, kg/s), cloud duration (t_c, s), cloud diameter (m)
- Jet liquid mass rate (Q_L, kg/s), jet liquid duration (t_L, s), jet vapor mass rate (Q_V, kg/s), jet vapor duration (t_V, s), jet diameter (m)
- Pool evaporation mass rate (Q_p, kg/s), pool evaporation duration (t_p, s), pool off-gassing mass rate (Q_o, kg/s), pool off-gassing duration (t_o, s), pool diameter (m)

There are five (5) possible source types:

- One (1) = horizontal plume vapor source
- Two (2) = constant area pool vapor source
- Three (3) = growing area pool vapor source
- Four (4) = constant area cloud vapor source
- Five (5) = growing area cloud vapor source

The first two (2) values in the second line include both vapor and aerosol, while the last two (2) values reflect the cloud density and concentration after all aerosol has evaporated. The file generated for the Jack Rabbit ammonia pilot test is shown in Figure 21.

```
      4      154.57         0.0      3302.6      0.2740
   1.3786    0.0274        1.70      1.3786      0.0274
 0.000020    252.64      0.2646      3302.6      154.57
  10.3742      73.5      1.5607        90.9        2.55
   0.0675     640.7      0.0169         0.0        9.58
```
Figure 21. Example RAILCALC.OUT

The source type for the example run is a constant area cloud vapor source. The tank empty time is very short compared to the cloud duration, so the source is defined as a constant area cloud vapor source, and the cloud growth duration is set to zero (0) seconds. The large air entrainment volume evaporates all aerosol, so the two (2) values for cloud concentration and density are the same.

The third through fifth lines provide additional source parameters which may be of use in an ATD model. Each line contains source terms for the stationary cloud, jet, and liquid pool, and allows for a more detailed source characterization than the simplified overall source type defined in the first line. The jet parameters in the fourth line provide the total source mass, M_j:

$$M_j = Q_L\, t_L + Q_V\, t_V \tag{5}$$

Both the stationary vapor cloud and liquid pool area grow linearly during the jet liquid duration. The stationary cloud parameters in the third line can be used with the jet liquid duration to compute vapor mass from the mist pool or stationary vapor cloud, M_c:

$$M_c = Q_c\, (t_c - 0.5\, t_L) \tag{6}$$

The liquid pool parameters in the fifth line can be used with the jet liquid duration to compute vapor mass from the boiling or evaporation liquid pool, M_p:

$$M_p = Q_p\, (t_L - 0.5\, t_L) + Q_o\, t_o \tag{7}$$

Cloud mass plus pool mass equals jet mass ($M_j = M_c + M_p$). The simplified overall source type defined in the first line will contain the diameter for one (1) of the source types, where the jet diameter is vertical rather than horizontal. The duration will be the sum of the jet liquid and vapor durations, cloud duration, or sum of pool evaporation and off-gassing durations. The vapor mass rate is adjusted to include all the mass in the simplified source. The growth duration is the total jet duration for the two (2) growing area source types. If there is foaming in the tank and much of the total mass released is during tank depressurization, the total jet duration should be used in Equations (6) and (7) in place of the jet liquid duration.

Key output parameters are displayed in the Output Window. The Output Window for the example run is shown in Figure 22.

Figure 22. Example Run Output Window

The user can print the output window or the output summary file from the Output Window. A standard Microsoft Windows print dialog window is displayed, as shown in Figure 23.
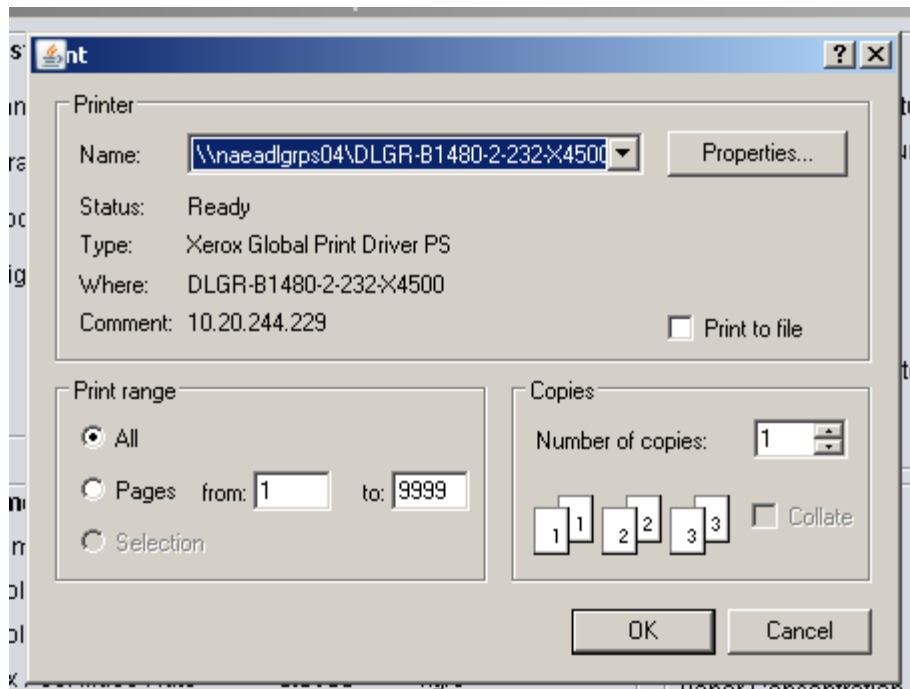
Figure 23. Print Dialog Window

The user exits the program by selecting Exit from the **File** pull-down menu displayed in Figure 24.
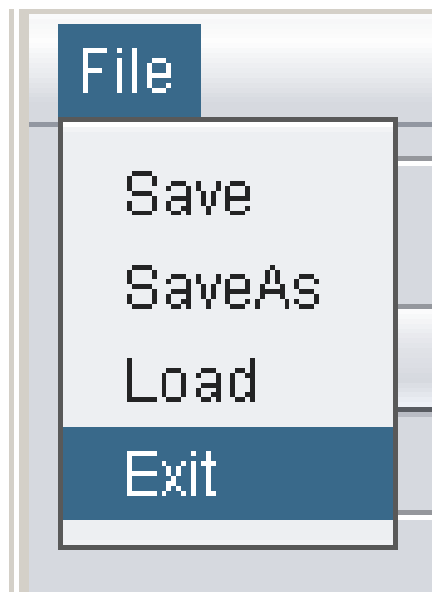
Figure 24. File Pull-Down Menu

3.6 Interpreting the Output File

The RAILCAR4.1 calculations are divided into the physical processes being simulated. The processes have times and durations associated with them, but RAILCAR4.1 does not use time steps. This section describes the processes and the information recorded to RAILCAR.OUT. The output associated with the input parameters contained in Figures 11, 14, and 15 for the Jack Rabbit ammonia pilot test addresses almost all of the relevant physical processes. The first output is a summary of some of the physical properties read from the thermodynamic property file for the TIC.

```
RAILCAR version 4.1

TIC released= ammonia

boiling temperature properties:
temperature=              -33.96 C
pressure=                   1.00 atm
liquid density=           681.00 kg/m3
vapor density=              0.87 kg/m3
heat of vaporization=    1372.00 kJ/kg
liquid heat capacity=       4.44 kJ/kg-K
vapor heat capacity=        2.29 kJ/kg-K

other physical properties:
molecular weight=          17.03 g/mole
freezing temperature=     -78.20 C
critical temperature=     132.40 C
liquid viscosity=           0.14 cp
surface tension=           26.40 dyne/cm
vapor diffusivity=          0.153 cm2/s
```

The physical properties are followed by a summary of the tank and meteorological conditions defined by the user.

```
initial mass=             907.0 kg
recovered liquid=           0.0 kg
air temperature=           -0.10 C
ground temperature=         0.70 C
tank temperature=          -0.50 C
relative humidity=         78.00%
terrain elevation=          0.00 m
ambient air pressure=     1.0000 atm
liquid head pressure=     0.0300 atm
inert head pressure=      2.1300 atm
ullage volume frac.=        0.60
tank thickness=           0.4100 m
```

If the tank temperature is above the TIC critical temperature, a message is recorded stating that the tank will have no remaining liquid.

The liquid head pressure algorithm is called if the liquid head pressure is not defined by the user. The tank thickness is also set by the program if not defined by the user. The density of air for the entered air temperature and relative humidity is computed, and the thermodynamic properties of the TIC are interpolated for the initial tank temperature. The physical properties for air and water vapor are stored internally to the program.

```
initial tank properties:
temperature=                -0.50 C
vapor pressure=              4.18 atm
pressure=                   6.31 atm
liquid density=           639.78 kg/m3
vapor density=              5.94 kg/m3
heat of vaporization=    1275.31 kJ/kg
water vapor pressure=      0.0058 atm
liquid mass=              900.2 kg
vapor mass=                6.77 kg
inert mass=                5.86 kg
```

The tank volume is computed from the initial mass, liquid density, and ullage volume fraction. The initial vapor mass is computed from the ullage volume fraction and tank temperature. The inert mass is calculated from the ullage volume fraction and tank temperature using the molecular weight of dry air. The final tank properties are estimated by adiabatically expanding the initial inert and TIC vapor from their partial pressures to ambient pressure; however, there will be considerable additional TIC vapor generated during depressurization and auto-refrigeration that does not need to be adiabatically expanded. The adiabatically expanded inert and TIC vapor and the TIC vapor generated are brought into thermal equilibrium using the masses and heat capacity values, and the final masses are computed.

```
final tank temp.=          -43.85 C
tank volume=                3.54 m3
vapor remaining=            2.12 kg
inert remaining=            1.84 kg
vapor density=              1.12 kg/m3
```

The liquid superheat equals the tank temperature minus the TIC boiling temperature. Based on literature data from small-scale tests releasing pressurized liquid, a superheat of less than about 20 °C will generate large droplets that fall to the ground, while a higher superheat will generate small droplets that remain suspended in the cloud or plume. The transition point is somewhat arbitrary and does not involve a step change, but it has been treated as such for simplicity. The jet is adiabatically expanded from the tank partial pressure to ambient with the liquid mass vaporized being determined by the energy required to cool the plume to the TIC boiling temperature. In addition to the equations included in Bauer and Fox[7], RAILCAR4.1 also

addresses work from expansion and the energy of the surface tension in the suspended droplets. If the tank temperature is below the TIC boiling temperature, the jet will be all liquid, and if the tank temperature is above the critical temperature, the jet will be all vapor.

```
liquid superheat=           33.46 C
20 micron droplets; droplets remain in cloud
aerosol rainout=            6.00%
jet is 10.88% vapor and 89.12% liquid
jet density=                7.89 kg/m3
```

Using the methodology described in Bauer and Fox[7] for the final tank conditions above and those at the point when the vapor-liquid interface reaches the hole, the behavior of the tank while the liquid is emptying is determined. As with the jet expansion algorithm, work from expansion is included in RAILCAR4.1. The inert vapor is also adiabatically expanded as the vapor space volume increases.

```
tank before depressurization:
temperature decrease=      5.00 C
liquid temperature=       -5.50 C
vapor temperature=       -10.80 C
tank pressure=             4.69 atm
vapor pressure=            3.46 atm
liquid density=          645.94 kg/m3
vapor density=             4.46 kg/m3
heat of vaporization=   1289.76 kJ/kg
vapor mass=                9.0 kg
liquid mass=               0.0 kg
vapor mass generated=      6.9 kg
enthalpy before=        1.9029E+04 kJ
enthalpy after=         1.9949E+04 kJ
enthalpy difference=   -9.2007E+02 kJ
```

For the Jack Rabbit ammonia pilot test, the liquid temperature is predicted to decrease by almost five (5) °C, but the vapor above it is estimated to be more than five (5) °C colder. The vapor mass generated is the mass of liquid vaporized while the liquid empties, based on the liquid temperature. Some of this vapor will also exit the tank during the subsequent depressurization period to end at the final tank properties above. As mentioned in Section 2.5, RAILCAR4.1 appears to overestimate temperature decrease and underestimate pressure decrease. There were no thermocouples in the vapor spaces of the tanks in the Jack Rabbit pilot tests and field trials to confirm that the vapor was cooler than the liquid below.

The next set of algorithms address the behavior of the liquid and vapor jets. As already discussed, algorithms dealing with foaming of the liquid and vaporization in the liquid jet had to be added to the Bauer and Fox[7] methodology. For this example, a liquid foaming fraction

of 0.15 and a 0.035 vaporization fraction of the liquid jet resulted in agreement with the liquid empty time and tank depressurization time. The restrictor orifice was used in this case. The hole or pipe properties and foaming and vaporization parameters are output.

```
hole/pipe area=          0.00811 m2
hole/pipe diameter=         4.00 in
orifice area=            0.00203 m2
orifice diameter=           2.00 in
foaming occurs
liquid fraction foam=     0.1500
min. frac. vaporized=     0.0350
```

Properties for the jet are broken into three (3) output times. The jet properties at the initial tank conditions are computed, followed by the jet properties when the vapor-liquid interface reaches the hole. The vapor jet properties immediately after that point are then computed. The final vapor jet has a mass flow rate of zero (0) due to the depressurization and auto-refrigeration. For simplicity, the average of the liquid jet properties can be used, and the vapor mass flow rate can be considered half of the value at the start of depressurization. The liquid jet flow rate will likely decrease close to linearly, but the vapor jet may be more asymptotic. Checks on the flow equations are included to prevent the jet velocity from exceeding the speed of sound (i.e., choked flow) for liquid, vapor, or two-phase flow. For this example, the liquid empty time is estimated to be 35 seconds, followed by a 41-second depressurization time.

```
initial jet properties:
fraction vaporized=       0.0350
liq. speed of sound=   1804.43 m/s
liquid jet is not choked
jet velocity=             78.49 m/s
jet density=              63.14 kg/m3
pressure drop=            0.0072 atm
Reynolds number=        8.9922E+05
mass flow rate=           10.05 kg/s
final jet properties:
fraction vaporized=       0.0350
liq. speed of sound=   1795.88 m/s
liquid jet is not choked
jet velocity=             63.70 m/s
jet density=              82.89 kg/m3
pressure drop=            0.0051 atm
Reynolds number=        9.5805E+05
mass flow rate=           10.70 kg/s
average jet properties:
average jet velocity=     71.10 m/s
avg. mass flow rate=      10.37 kg/s
liquid mass expulsed=     763.0 kg
liquid empty time=        73.5 s
```

```
initial vapor jet properties:
foam speed of sound=   1693.68 m/s
vapor jet is not choked
jet velocity=            169.96 m/s
jet density=               9.32 kg/m3
pressure drop=           0.0050 atm
Reynolds number=         2.8733E+06
mass flow rate=            3.12 kg/s
average velocity=         84.98 m/s
average flow rate=         1.56 kg/s
vapor mass expulsed=      141.9 kg
inert mass expulsed=       4.02 kg
depress. time=            90.9 s
combined jet properties:
avg. mass flow rate=       5.50 kg/s
tank empty time=          164.5 s
```

If the jet is all-vapor, no liquid jet output is recorded, and an all-liquid jet will have no vapor jet output. If a liquid pool is determined to form or is specified by the user to reflect rainout due to ground impaction of the jet, the characteristics of the pool are simulated. The mist pool methodology of Bauer and Fox[7] does not address liquid pool evaporation. The pool evaporation algorithm in RAILCAR4.1 is that used by the Chemical and Biological Agent Vapor, Liquid, and Solid Tracking (VLSTRACK) hazard prediction model for evaporation of chemical agent deposited onto various ground surfaces.[36]

$$q_p = 10^{-7} \, Sh \, D \, P_v \, M_w/(8.206E\text{-}5 \, T_a \, L) \tag{8}$$

Where q_p is the vapor flux in kg/m^2-s, Sh is the Sherwood number based on the Reynolds and Schmidt numbers for the surface wind, D is the vapor diffusivity in cm^2/s, P_v is the vapor pressure in atm, M_w is molecular weight in g/mole, T_a is air temperature above the pool in °K, and L is a length scale in meters. Conversion constants are included, since the units of measurement are mixed. This equation is based on mass transfer to passing air being the limiting process, which is not necessarily appropriate for high-volatility liquids where heat transfer is the limiting process. Since the characteristics of the surface materials, which determine the amount of heat available, will not be known, the mass transfer equation is used with the vapor pressure of the liquid at the pool temperature. The pool temperature is set equal to the ground temperature for liquids having a boiling temperature above the ground temperature (an evaporating liquid pool) and the boiling temperature for liquids generating a boiling liquid pool. The other physical properties in Equation (5) are computed at the average of the pool temperature and the two (2)-m air temperature. This approach is very limited but did result in good agreement with the Jack Rabbit field trial pool evaporation durations. The VLSTRACK pool evaporation predictions can be considered reasonably accurate for chemicals stored at temperatures below their boiling temperatures but only rough estimates for boiling liquid pools.

The pool evaporation algorithm accounts for vapor mass lost during the liquid empty period to determine the pool area, which is then assumed constant for the remaining pool evaporation duration:

$$A_p = (Q/q_p) [1 - exp(-q_p t/(\rho_L H_p)] \qquad\qquad [9]$$

where A_p is the pool diameter, ρ_L is the liquid density, and H_p is the pool thickness.

```
pool evaporation:
pool temperature=         -33.96 C
liquid pool depth=         0.0780 cm
wind speed at 2 m=          0.30 m/s
mass frac. absorbed=       0.0000
total pool mass=           40.80 kg
pool diameter=              9.58 m
(equals diameter at tank jet empty time)
formation vapor rate=    3.3774E-02 kg/s
final pool area=           72.13 m2
mass for final area =      38.31 kg
final vapor rate=        6.7548E-02 kg/s
combined vapor rate=     6.3671E-02 kg/s
combined evap. time=      640.72 s
```

If liquid off-gassing occurs due to absorption of liquid into the ground surface, the time at which the mass fraction in the surface liquid is gone is computed. The remaining liquid within the ground surface is then assumed to off-gas at a rate equal to 25% of the pool evaporation rate. Key output for pool evaporation includes the pool diameter at the tank empty time, the evaporation rates during formation, evaporation, and off-gassing, and the durations for evaporation and off-gassing. Pool durations are limited to 24 hours for output formatting reasons.

If the chemical is stored below its boiling temperature, no mist pool or stationary cloud will form. The message

```
no mist pool forms
```

is displayed, and the simulation skips the cloud property computations; otherwise, the simulation moves to the mist pool algorithms. The mass considered for the mist pool formation criterion includes the mass from the liquid jet, the chemical and inert mass from tank depressurization, the air entrained into the jet, and the vapor from pool evaporation during the tank empty time. This last mass is computed from the pool evaporation rates and the tank empty time. Before plugging values into the mist pool criterion in Equations (1) to (3), a determination needs to be made as to whether the cloud will contain aerosol (a mist pool) or will be all vapor (a stationary vapor cloud) from the entered volumetric air entrainment ratio. RAILCAR4.1 contains an algorithm that determines the air entrainment ratio at which point all

aerosol evaporates. This point is also the coldest potential cloud temperature, as the aerosol evaporation removes energy from the cloud without any additional energy being added by excess air. If the source is all-vapor or no aerosol is present due to rainout or jet expansion, the message

```
no liquid aerosol present in cloud
entrainment volume to evaporate aerosol equals 0
```

is displayed. Determining the maximum entrainment ratio requires an iterative process on the cloud temperature. Cloud cooling from aerosol can lead to temperatures well below the chemical boiling temperature, but the cloud temperature is not allowed to drop below the chemical freezing temperature. A message is displayed if the temperature iterations reach the freezing temperature:

```
temperature reset to freezing temperature
```

The properties at the maximum entrainment ratio are then determined.

```
entrainment ratio=          290.00
maximum entrainment ratio=  80.76
minimum cloud temperature= -71.57 C
equilibrium vapor press.=    0.11 atm
```

If the entered entrainment ratio is equal to or below the maximum entrainment ratio, a mist pool will form if the criterion is met. If the entered entrainment ratio is above the maximum entrainment ratio, a stationary vapor cloud will form if the criterion is met.

The cloud temperature, density, concentration, and diameter are needed for the mist pool formation criterion. The next set of algorithms then applies the mist pool methodology for homogeneous equilibrium to determine the cloud properties for the masses described above. Other than the cloud diameter and height, the cloud temperature, density, and concentration characterize the plume following adiabatic expansion, air entrainment, and homogeneous equilibrium if the mist pool criterion is not met. The methodology defined by Bauer and Fox[7] has been extended to allow for complete aerosol evaporation and subsequent cloud warming resulting from a volumetric air entrainment ratio exceeding the maximum entrainment ratio computed in the previous algorithm. A similar iterative solution on temperature to the maximum entrainment ratio algorithm is used for the cloud property algorithm, so the same limit on freezing temperature is applied and uses the same display message. RAILCAR4.1 outputs a summary of the properties calculated for the mist pool, stationary cloud, or plume that includes the cloud temperature, density, and concentration. The plume diameter is needed to characterize the source if a mist pool or stationary cloud is not formed. The diameter represents the plume after the jet has equilibrated with the entrained air.

```
final cloud properties:
temperature=                -20.51 C
heat of vaporization=   1333.13 kJ/kg
water fraction not freezing=  0.47932
aerosol evaporation fraction= 1.00000
partial pressure=        0.0333 atm
saturation pressure=     1.8636 atm
water vapor pressure=    2.1626E-03 atm
ambient water vapor fraction= 0.00281
ambient air density=     1.2903 kg/m3
dry air density=         1.2867 kg/m3
water vapor density=     0.0036 kg/m3
cloud liquid density=    664.43 kg/m3
cloud density=           1.3786 kg/m3
cloud concentration=     0.0274 kg/m3
cloud is 1.07 times that of air
plume diameter=            2.55 m
```

The final set of algorithms includes the mist pool criterion and the mist pool methodology for releases meeting the criterion. The Richardson number of the cloud after assumed formation is computed using Equation (3) and displayed and recorded. A mist pool cannot form if the Richardson number is for neutral conditions ($Ri_* = 0$) or positively buoyant ($Ri_* > 0$), so a message is displayed if either condition exists:

```
   mist pool will not form
```

at which point the cloud property computations are complete; otherwise, the ratio of vapor mass entrainment rate over jet mass flow rate (i.e., mist pool ratio) is computed, displayed, and recorded. The same message is displayed if the ratio is greater than or equal to one (1), and the cloud property computations are again complete. In order to avoid unrealistically low vapor mass entrainment rates, the Richardson number for the mist pool criterion and the following mist pool behavior equations is limited to a value of 100. If the mist pool ratio is less than one (1), RAILCAR4.1 computes and outputs the total mass, chemical mass, liquid mass, and vapor mass in what will now be either a mist pool or a stationary cloud. A chemical liquid mass of zero (0) kg, as in the example below, signifies that no aerosol is present, and the cloud is a stationary vapor cloud.

```
cloud height=              1.70 m
friction velocity=       0.0160 m/s
cloud Richardson number= 4458.4
entrainment factor=        0.24
mist pool ratio=         0.0052
cloud mass=            43982.0 kg
chemical mass=          872.7 kg
chemical liquid mass=     0.0 kg
chemical vapor mass=    872.7 kg
```

If a liquid pool forms, the chemical mass will not equal the difference of the initial mass minus the final mass remaining in the tank minus the pool mass. For the pool evaporation summary above, the "total pool mass" equals all of the liquid that rains out of the jet onto the ground surface. Some liquid evaporates while the pool forms during the liquid jet duration. The resulting mass is provided as the "mass for final area" and that mass is added to the mist pool/stationary cloud mass. However, additional vapor is generated from pool evaporation as the tank depressurizes. This mass equals the "final vapor rate" for the pool times the "depress. time" for the vapor jet. This mass is also added to the mist pool/stationary cloud mass. A mass balance between the initial tank, final tank, liquid pool, and mist pool/stationary cloud must subtract this additional vapor mass from the pool mass to be correct.

RAILCAR4.1 then proceeds to compute the properties of the mist pool or stationary vapor cloud at each of the stages defined in Section 2. The first stage involves formation of the mist pool during the tank empty time, which includes the time for tank depressurization. Although vapor mass is entrained by passing air during this stage, Bauer and Fox[7] do not adjust the cloud diameter for the mass lost during cloud formation. As with the liquid pool formation, RAILCAR4.1 accounts for vapor mass lost during the tank empty period to determine the cloud area, which is then assumed constant for the remaining mist pool/stationary vapor cloud duration:

$$A_c = (Q_f/q_{v1}) \, [1 - exp(-q_{v1} \, (t + t_d)/(\rho_c \, H_c)] \qquad [10]$$

where A_c is the cloud diameter, Q_f is the average jet mass flow rate for the liquid empty time plus depressurization time, q_{v1} is the vapor flux in kg/m^2-s, t_d is the tank depressurization duration, ρ_c is the cloud density, and H_c is the cloud thickness. If there is no aerosol present in the cloud, the message

```
no aerosol present; stage 2 skipped
```

is displayed. If it is determined that there is aerosol retained in the jet, but the aerosol evaporates from air entrainment, the message

```
all aerosol will evaporate while the tank empties
stage 2 skipped
```

is displayed. Since Stage 2 involves evaporation of the aerosol within the cloud after formation, there will be no Stage 2 output. If the Richardson number at the end of Stage 1 or Stage 2 becomes less than or equal to zero (0), the message

```
cloud becomes buoyant after aerosol evaporation
```

is displayed, and no Stage 3 calculations are done. If the Richardson number at the beginning of Stage 3 is less than or equal to 12, the message

```
     Richardson number is not greater than 12
     so no part 1 of stage 3
```

is displayed, and only the second part of Stage 3 is computed. RAILCAR4.1 then outputs the entrainment rate and duration for each stage, along with the average entrainment rate and total duration for the combined mist pool or stationary vapor cloud behavior. The duration of Stage 1 equals the tank empty time, which was already an output from the jet algorithms and is not repeated here.

```
     sheltering factor=      4.1
     stage 1 entrainment:
     entrainment rate=        0.0288 kg/s
     no aerosol present; stage 2 skipped
     final cloud diameter=    154.57 m
     stage 3 entrainment:
     stage 3, part 1 entrainment:
     entrainment rate=        0.2683 kg/s
     duration=                3226.6 s
     stage 3, part 2 entrainment:
     frac. at Ri eq. 12=      0.0027
     entrainment rate=        0.9406 kg/s
     duration=                   2.5 s
     average entrainment values:
     entrainment rate=        0.2642 kg/s
     mist pool duration=      3302.6 s
```

The final part of the mist pool algorithm is an assessment of the durations of the jet, liquid pool, and mist pool/stationary vapor cloud. Transport and diffusion models normally handle only a single source type, so this part of the algorithm identifies which of the three (3) processes dominate and should be used for model input. If the mist pool duration is less than or equal to the liquid pool duration and the liquid mass in the pool is more than 50% of the release mass, the message displayed is

```
     mist pool duration less than liquid pool duration
```

RAILCAR4.1 then adds the mist pool mass to the liquid pool mass and computes the new average vapor rate for the liquid pool duration.

If the mist pool duration is within 10% of the tank empty time, the initial source will be a plume having the diameter output with the final cloud properties. The message displayed is

```
     mist pool duration is similar to tank empty time
```

The liquid pool will still be the dominant source if the criteria above are met. A plume should only form from a pressurized liquid for a chemical stored at a temperature above its boiling temperature. Other chemicals should form a liquid pool. Adiabatic expansion of the jet with a low air entrainment ratio such as five (5) will lead to a plume diameter approximately 20 times the hole diameter. Adiabatic expansion of the jet with a high air entrainment ratio such as 100 will lead to a plume diameter approximately 100 times the hole diameter. All-vapor TICs do not expand from liquid evaporation, so the plume diameter will be due to adiabatic vapor expansion and air entrainment. The low air entrainment ratio and high air entrainment ratio plume diameters become approximately two (2) and 10 times the hole diameter, respectively.

If the mist pool duration is between 1.1 and five (5) times the tank empty time, the message displayed is

```
mist pool area versus time must be considered
```

The cloud will grow from zero (0) to the diameter output for the tank empty time, with the vapor rate increasing linearly with cloud diameter to the value output for Stage 1. The vapor rate after cloud formation will follow the values output for Stages 2 and 3. If the mist pool duration is at least five (5) times the tank empty time, which is the case for the ammonia example, the message displayed is

```
mist pool can be assumed to form instantaneously
```

If no mist pool forms, the source type(s) will be a plume and/or a liquid pool.

After all of the physical property computations are completed, a summary of key predicted source properties is presented:

```
Source Characterization Summary:
final tank temp.=         -43.85 C
depress. temperature=      -5.50 C
depress. pressure=          4.69 atm
liquid empty time=         73.5 s
liquid jet flow rate=      10.37 kg/s
tank empty time=          164.5 s
avg. jet flow rate=         5.50 kg/s
plume diameter=             2.55 m
pool diameter=              9.58 m
pool duration=            640.7 s
max. pool mass rate=      0.0675 kg/s
off-gassing duration=     640.7 s
avg. pool mass rate=      0.0637 kg/s
cloud diameter=           154.57 m
cloud temperature=        -20.51 C
vapor density=            1.3786 kg/m3
```

```
vapor concentration=        0.0274 kg/m3
cloud duration=             3302.6 s
cloud vap. mass rate=       0.2642 kg/s
```

RAILCAR4.1 then determines the most appropriate source type of plume vapor source or area vapor source, and the simplified vapor source properties of diameter, duration, and mass rate are presented. The diameter, duration, and mass rate for the other source type are all set to zero (0).

```
Constant Area Vapor Source Properties:
diameter=                   154.57 m
duration=                   3302.6 s
vapor mass rate=            0.2740 kg/s
height=                       1.70 m
```

The output for the Jack Rabbit ammonia pilot test used as an example can now be interpreted for input into a hazard assessment model for either sophisticated source characterization or simple source characterization. The test has a tank empty time of 164.5 seconds. The liquid jet lasts 73.5 seconds at a mass flow rate of 10.37 kg/s. Adding in the two-phase jet from depressurization decreases the mass flow rate to 5.50 kg/s. The diameter of the jet if no mist pool or stationary vapor cloud is formed is 2.55 meters. The pool evaporation duration is 640.7 seconds. The pool diameter grows to 9.58 meters over the 164.5-s tank empty time, at which point the pool vapor mass rate equals 0.0675 kg/s. No liquid absorbs into the ground, so there is no off-gassing duration. Accounting for the lower vapor flux of the liquid pool as it grows to its final diameter results in an average pool vapor mass rate of 0.0637 kg/s. The stationary cloud duration is 3302.6 seconds; note that RAILCAR4.1 output uses the term "mist pool" even if no aerosol is present, as in this case. The stationary vapor cloud grows to a diameter of 154.57 meters over the 164.5-s tank empty time. The average vapor mass rate from the stationary cloud is 0.2642 kg/s.

At the point when depressurization in the tank begins, the temperature of the liquid in the tank is -5.5 °C, and the pressure is 4.69 atm. The temperature in the tank when it becomes empty is -43.9 °C. The temperature of the stationary cloud is -20.5 °C. Since the stationary cloud has the longest duration, it is the dominant source. The release height for the area vapor source is the 1.7-m cloud height. The simplified properties for the area vapor source include the stationary cloud diameter of 154.57 meters and duration of 3302.6 seconds. Adding the additional vapor mass to the stationary cloud results in a vapor mass rate of 0.2740 kg/s.

3.7   Operation by a Hazard Assessment Model

The RAILCAR4.1 computations were organized into a FORTRAN 77 subroutine named RAILCALC that can be called by a hazard assessment model. The hazard assessment model must pass in all the input parameters and the TIC physical properties, and RAILCAR4.1 will return the plume or cloud diameter, duration, and vapor flux, and the other summary parameters described in Section 3.6. RAILCAR4.1 also provides the atmospheric properties and constants it defined in case they can be used by the hazard assessment model. A simpler approach is to operate RAILCAR4.1 by having the hazard assessment model spawn the GUI Java file, Railcar.jar, or the RAILCALC executable, railcalc.exe. The hazard assessment model must generate the input file, railcalc.dat, if the latter approach is used. If the GUI is used, the user simply defines the incident the same as using RAILCAR4.1 as a stand-alone program. The source is defined in the output file, RAILCALC.OUT, which can be read by the hazard assessment model.

3.8   Subroutine Structure and Function

The parameters used within RAILCALC are defined in Table 5.

Table 5. RAILCALC Parameter Definitions

Input Parameters

a2	Orifice area in m^2
aj	Hole/pipe area in m^2
anta	Antoine constant A for temperature in C and pressure in atm
antb	Antoine constant B for temperature in C and pressure in atm
antc	Antoine constant C for temperature in C and pressure in atm
cplb	Chemical liquid heat capacity at boiling temperature in kJ/kg-K
cpvb	Chemical vapor heat capacity at boiling temperature in kJ/kg-K
d2	Orifice diameter in inches
dd	Equivalent hole/pipe diameter in inches
delhv	Heat of vaporization rate of change with temperature in kJ/kg-K
delrhol	Liquid density rate of change with temperature in kg/m^3-K
dif	chemical vapor diffusivity at 20 C in cm^2/s
ec	Entrainment ratio
ent	Entrainment factor
	1= enhanced
	2= normal
	3= sheltered
frain	Aerosol fraction rained out due to impaction
hc	Cloud height in m
headtp	Liquid head pressure mode
	0= calculated
	1= user input
hp	Liquid pool depth in cm
hsize	Hole/pipe parameter type
	1= area
	2= diameter
	3= small hole
	4= large hole
	5= rupture
	6= large rupture
	7= very large rupture
hvb	Chemical heat of vaporization at boiling temperature in kJ/kg
ifoam	Does foaming occur?
	0= no
	1= yes
ll	Tank thickness in m
minp	Mass input type
	0= mass
	1= chlorine tank size
mr	Recovered liquid mass in kg
mt	Initial tank mass in kg
mw	Chemical molecular weight in g/mole
otype	Orifice type
	0= unrestricted
	1= restricted
phead	Liquid head pressure in atm
pinert	Inert gas head pressure in atm
pt0	Tank pressure in atm
rh	Percent relative humidity
rholb	Chemical liquid density at boiling temperature in kg/m^3
sfac	Sheltering factor

Table 5. RAILCALC Parameter Definitions (Continued)

sunits	Terrain elevation type
	0= surface height
	1= surface pressure
	2= all-vapor, instantaneous release (e.g., Thorney Island)
shght	Surface height in m
sigma	Chemical liquid surface tension at boiling temp. in dynes/cm
tair	Air temperature in °C
tanktp	Tank thickness input type
	0= user input
	1= default
tcrit	Chemical critical temperature in °C
tfrz	Chemical freezing temperature in °C
tgrnd	Ground temperature in °C
ticname	TIC name
ttic	Tank temperature in °C
ufrac	Ullage volume fraction
ustar	Friction velocity in m/s
uvel	Wind speed at 2 m height in m/s
vis	Chemical liquid viscosity at 20 °C in cp
xfoam	Percent liquid fill becoming foam
xmin	Minimum vaporization percent
xoff	Pool mass fraction absorbing into ground

Output Parameters

conDia	Area vapor source diameter in m
conf	Plume/cloud vapor concentration in kg/m^3
conHt	Area vapor source height in m
conRate	Area vapor source mass rate in kg/s
conTime	Area vapor source duration in s
cpa	Heat capacity of air in kJ/kg-K
cpwl	Heat capacity of water in kJ/kg-K
cpws	Heat capacity of ice in kJ/kg-K
cpwv	Heat capacity of water vapor in kJ/kg-K
dc	Cloud diameter in m
delcpl	Liquid heat capacity slope with temperature in kJ/kg-K
delcpv	Liquid heat capacity slope with temperature in kJ/kg-K
dp	Plume diameter in m
dpool	Pool diameter in m
hfw	Heat of fusion of water in kJ/kg
hvw	Heat of vaporization of water in kJ/kg
insDia	Plume vapor source diameter in m
insRate	Plume vapor source mass rate in kg/s
insTime	Plume vapor source duration in s
mwa	Molecular weight of air in g/mole
mww	Molecular weight of water in g/mole
pb	Ambient air pressure in atm
pd	Depressurization pressure in atm
pi	Rotational constant pi
qj	Liquid jet mass flow rate in kg/s
qpf	Average pool vapor mass rate in kg/s
qpool	Maximum pool vapor mass rate in kg/s
qv	Cloud vapor mass rate in kg/s
qvavg	Average mass flow rate in kg/s
qvt	Final growing pool/cloud mass rate in kg/s

Table 5. RAILCALC Parameter Definitions (Continued)

```
rg          Ideal gas constant in m3-atm/mole-K
rhof        Plume/cloud vapor density in kg/m³
rhows       Density of ice in kg/m³
srctp       final source type
            1 = horizontal plume vapor source
            2 = constant area pool vapor source
            3 = growing area pool vapor source
            4 = constant area cloud vapor source
            5 = growing area cloud vapor source
tb          Chemical boiling temperature in °K
tbn         Chemical normal boiling temperature in °K
tc          Cloud temperature in °K
td          Depressurization temperature in °K
tdur        Cloud duration in s
tevap       Off-gassing duration in s
tf          Liquid empty time in s
tfw         Freezing temperature of water in °K
tpool       Pool duration in s
tr          Final tank temperature in °K
tref        temperature unit of conversion from °C to °K
tv          Tank empty time in s
```

The structure and function of subroutines contained in the RAILCAR4.1 source code follows.

main—manages the RAILCAR4.1 program
      Subroutines called:
            readrail
            chemprop
            airprops
            propint
            h2oint
            hprops
            liqadj
            headp
            ftank
            depress
            jet
            poolevap
            entmax
            cltemp
            mistpool
readrail—reads the input parameters from the specified input file
      Called by:
            main

chemprop—reads the thermodynamic properties from the specified TIC file
> Called by:
>> main

airprops—defines physical properties for moist air and standard constants
> Called by:
>> main

propint—linearly interpolates TIC saturation properties to the entered temperature
> Called by:
>> main
>> ftank
>> depress
>> poolevap
>> entmax
>> cltemp

h2oint—defines and interpolates saturation properties for water to the entered temperature
> Called by:
>> main
>> entmax
>> cltemp

hprops—defines the hole diameter, area, and angle for 5 representative hole types
> Called by:
>> main

liqadj—adjusts recovered mass for vapor mass generated by venting
> Called by:
>> main

headp—calculates the liquid height and head pressure in the tank using a standard aspect ratio
> Called by:
>> main

ftank—calculates the temperature and masses in the tank after depressurization
> Called by:
>> main
> Subroutines called:
>> expand
>> propint

expand—adiabatically expands vapor from one temperature and pressure to another
> Called by:
>> ftank

depress—solves energy balances to determine the tank conditions when depressurization begins
> Called by:
>> main
> Subroutines called:
>> propint

jet—estimates initial and final liquid jet properties and initial vapor jet properties

  Called by:

    main

poolevap—computes the vapor flux and diameter of a boiling or evaporating liquid pool

  Called by:

    main

  Subroutines called:

    propint

entmax—determines the maximum air entrainment ratio and cloud properties for aerosol survival

  Called by:

    main

  Subroutines called:

    propint

    h2oint

cltemp—estimates the cloud properties after jet expansion and air entrainment

  Called by:

    main

  Subroutines called:

    propint

    h2oint

mistpool—determines if a mist pool will form and the subsequent cloud behavior

  Called by:

    main

4   CONCLUSIONS

NSWCDD is leading the way in improving hazard assessment modeling capabilities for TIC incidents. As a result of the validation of the NSWCDD mist pool theory, in conjunction with the extensive measurements taken during the Jack Rabbit pilot tests and field trials, hazard assessment models will be better equipped to predict the downwind effects for emergency responders, and warfighters will be much better protected from these types of attacks. The RAILCAR4.1 program provides the best source characterization for incidents involving release of pressurized liquids under low to moderate wind speeds, especially in the presence of buildings, vegetation, and/or terrain undulations. RAILCAR4.1 can be operated as a stand-alone program, or the calculations can be done from another program by initiating the RAILCAR4.1 user interface or by generating input file railcalc.dat and executing railcalc.exe. Validation of the RAILCAR4.1 program with data from future field trials will provide confidence that the source characterization is accurate.

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